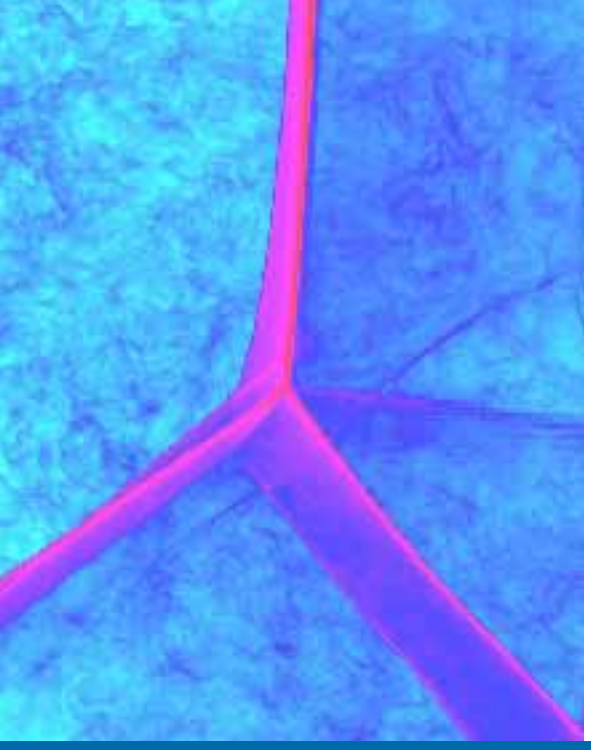
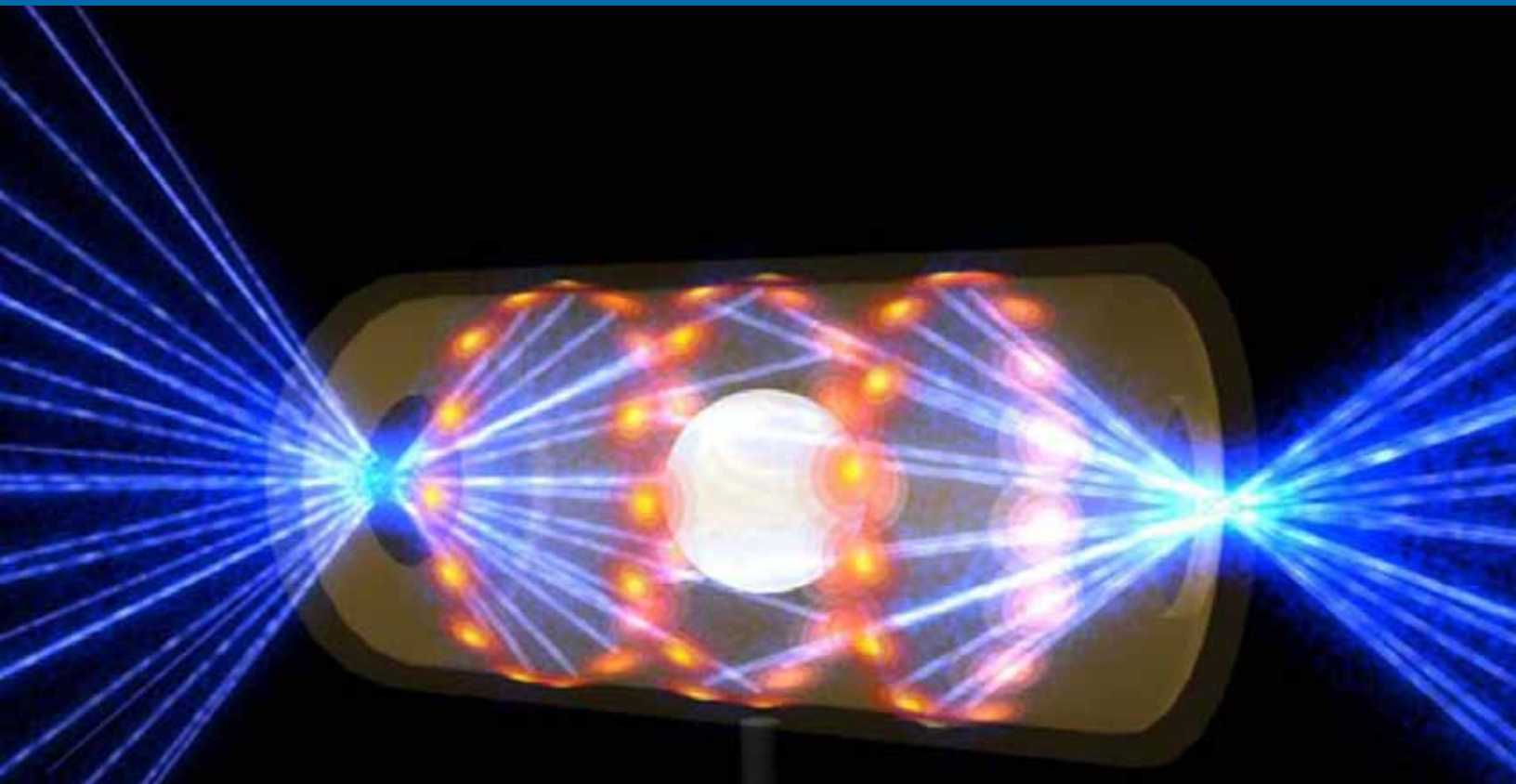


Argonne NATIONAL LABORATORY

Argonne Leadership Computing Facility

Argonne Leadership Computing Facility

extending the frontiers of science



2010 Science Highlights

February 2011

On the cover:

(Top) Three-dimensional Navier-Stokes first-principles direct numerical simulation of a Mach=3 reflected shock bifurcation in a hydrogen-oxygen mixture in a square channel, performed within the high-speed combustion and detonation project (HSCD). Pseudo-schlieren image of a temperature field. Credits: Alexei Khokhlov (U of C), Charles Bacon (ANL), Shashi Aithal (ANL), Joanna Austin (UIUC).

(Bottom) NIF Hohlraum. This artist's rendering shows a NIF target pellet inside a hohlraum capsule with laser beams entering through openings on either end. The beams compress and heat the target to the necessary conditions for nuclear fusion to occur. Ignition experiments on NIF will be the culmination of more than 30 years of inertial confinement fusion research and development, opening the door to exploration of previously inaccessible physical regimes. Credit: Lawrence Livermore National Laboratory.

Argonne Leadership Computing Facility Vision

The ALCF strives to be the forefront computational center for extending the frontiers of science by solving key problems for the nation that require innovative approaches and the largest-scale systems.

Second printing February 2011

CONTENTS

Argonne Leadership Computing Facility

Forefront Computational Center in Extending Science Frontiers

Several initiatives enable bold research that ventures into unexplored science frontiers at the Argonne Leadership Computing Facility (ALCF). The Innovative and Novel Computational Impact on Theory and Experiment (INCITE), ASCR Leadership Computing Challenge (ALCC), Early Science, and Director's Discretionary programs all provide avenues for scientists to conduct breakthrough science and engineering.

Innovative and Novel Computational Impact on Theory and Experiment (INCITE) Program

ALCF resources are available to researchers as part of the U.S. Department of Energy's INCITE program. Established in 2003, the program encompasses high-end computing resources at Argonne and other national laboratories. The INCITE program specifically seeks out computationally intensive, large-scale research projects with the potential to significantly advance key areas in science and engineering. The program encourages proposals from universities, other research institutions, and industry. It continues to expand, with current research applications in areas such as chemistry, combustion, astrophysics, genetics, materials science and turbulence.

ASCR Leadership Computing Challenge Program (ALCC)

Open to scientists from the research community in academia and industry, the ALCC program allocates resources to projects with an emphasis on high-risk, high-payoff simulations in areas directly related to the Department's energy mission, national emergencies, or for broadening the community of researchers capable of using leadership computing resources. Projects are awarded an ALCC allocation based on a peer review for scientific merit and computational readiness.

Early Science Program (ESP)

Allocations through the Early Science Program (ESP) provide researchers with preproduction hours (between system installation and full production) on the ALCF's next-generation, 10-petaflops IBM Blue Gene system. This early science period provides projects with a significant head start for adapting to the new machine and access to substantial computational time. During this shakedown period, users assist in identifying the root causes of any system instabilities, and work with ALCF staff to help develop solutions. More than four billion core hours are allocated through ESP.

Discretionary Projects

Discretionary allocations are "start up" awards made to potential future INCITE projects. Projects must demonstrate a need for leadership-class resources. Awards may be made year round to industry, academia, laboratories and others, and are usually between three and six months in duration. The size of the award varies based on the application and its readiness/ability to scale; awards are generally from the low tens of thousands to the low millions of hours.

Aerodynamics

Petascale, Adaptive CFD

The aerodynamic simulations proposed will involve modeling of active flow control based on synthetic jet actuation that has been shown experimentally to produce large-scale flow changes (e.g., re-attachment of separated flow or virtual aerodynamic shaping of lifting surfaces) from micro-scale input (e.g., a 0.1 W piezoelectric disk resonating in a cavity alternately pushes/pulls out/in the fluid through a small slit to create small-scale vortical structures that interact with, and thereby dramatically alter, the cross flow). This is a process that has yet to be understood fundamentally. Synthetic jet actuators offer the prospect of not only augmenting lift but also other forces and moments in a dynamic and controlled fashion for a range of operating conditions. They have been demonstrated to restore and maintain flow attachment and reduce vibrations in wind turbine blades during dynamic pitch, thereby reducing unsteady loads on gearboxes that are currently the prime failure point. In virtual-shape flight control surfaces for aerial vehicles (including commercial airplanes), conventional control surfaces (e.g., flaps, rudder, etc.) can be augmented or even replaced with active flow control, thus improving their lift-to-drag ratio and/or control power. This project's numerical simulations will give a detailed view of the flow interactions at a Reynolds number and simulation volume approaching engineering application scales for the first time. In these fluid flow problems, anisotropic solution features (like strong boundary and shear layers) can only be located and resolved through adaptivity of the computational mesh.

Early Science Program
Intrepid Allocation:
2 Million Hours

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Astro/Cosmology

Cosmic Structure Probes of the Dark Universe

Early Science Program
Intrepid Allocation:
6 Million Hours

Dark matter and dark energy are the dominant components of the Universe. Their ultimate nature, however, remains mysterious, especially so of the dark energy. Ambitious ground and space-based missions investigating different aspects of the "Dark Universe" constitute a national and international investment measured in billions of dollars. The discovery potential of almost all of these missions relies crucially on theoretical modeling of the large-scale structure of the Universe. As observational error estimates for various cosmological statistics edge towards the one percent level, it is imperative that simulation capability be developed to a point that the entire enterprise is no longer theory-limited.

This project is a simulation framework powerful enough to discover signatures of new physics from next- generation cosmological observations. Relevant questions include: (1) Beyond the cosmological constant, what are the detectable signatures of a dynamical equation of state for dark energy? (2) How does modification of general relativity alter the nonlinear regime of structure formation? As for dark matter and related questions: (1) What are the effects of plausible dark matter candidates on the mass distribution? (2) What are the constraints on the neutrino sector from cosmological observations? In addition, the results of the simulations will be very useful for a range of astrophysical investigations, primarily in the areas of galaxy formation and the formation and evolution of galaxy groups and clusters. This is possible because the next generation, 10-petaflops IBM Blue Gene system will provide, at last, the computational power to resolve galaxy-scale mass concentrations in a simulated volume as large as state-of-the-art sky surveys. Researchers will generate numerically a mock galaxy catalog that will allow the determination of the effects of new physics on major cosmological observables.

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Astro/Cosmology

Petascale Simulations of Turbulent Nuclear Combustion

Type Ia (thermonuclear-powered) supernovae are important in understanding the origin of the elements and are a critical tool in cosmology. These explosions produce a significant fraction of the heavy elements in the universe, and are therefore important in understanding the origin of the elements of which planets and life on Earth are made. Observations using Type Ia supernovae as "standard candles" revealed that the expansion of the universe is accelerating, which led to the discovery of dark energy. Understanding dark energy ranks among the most compelling problems in all of physical science. Type Ia supernovae are one of the most promising tools for determining the properties of dark energy. This is the purpose of the simulations that the Flash Center will do as an early science user on the next-generation Blue Gene system. To be specific, the Center will use the FLASH code to carry out large-scale, 3-D simulations of two key physical processes in Type Ia supernovae that are not fully understood: (1) buoyancy-driven turbulent nuclear combustion, and (2) the transition from nuclear burning in the flamelet regime to distributed nuclear burning. The simulations will be the largest ever done. The number of grid points in them will exceed by a factor > 20 those in the simulations the Center has done to date on the ALCF's Blue Gene/P computer, Intrepid.

Early Science Program
Intrepid Allocation:
5 Million Hours

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Bio/Protein

NAMD - The Engine for Large-Scale Classical MD Simulations of Biomolecular Systems Based on a Polarizable Force Field

Biology, at the atomic and molecular level, is governed by complex interactions involving a large number of key constituents, including water, ions, proteins, nucleic acids, and lipid membranes. The goal of this project is to develop new technologies to simulate virtual models of biomolecular systems with an unprecedented accuracy. Large-scale molecular dynamics (MD) simulations based on atomic models play an increasingly important role in the life sciences. Success with MD simulations of large-scale biomolecular systems hinges on the accuracy of the potential function and the efficiency of the dynamic propagation algorithm for adequate sampling of motions.

This project is focused on the program NAMD, currently one of the most optimal and efficient programs to carry out classical simulations of biomolecular systems. To enhance the sampling efficiency beyond that of brute-force MD simulations, researchers propose to implement several advanced strategies based on multiple copies such as replica-exchange MD (REMD) and/or Hamiltonian tempering (H-REMD). Because the quality and accuracy of the potential function (force field) is critical for meaningful MD simulations, the researchers will implement a new force field that incorporates the effect of induced polarization. They will carry out simulations covering a wide range of canonical and non-canonical DNA and RNA molecules for which a wealth of experimental data is available. In the case of the structures determined via X-ray crystallography, simulations will be performed in solution as well as in the crystal environment allowing for the impact of crystal contacts on the simulated structure and dynamics. The researchers will examine the performance of the new force field for a suite of key problems where induced polarization is anticipated to be critical. Work will include calculation of pKa shifts in selected proteins, redox potentials, cooperative binding of Ca2+ to the EF-hands in calbindin D9k, and interfacial potentials of lipid monolayers and bilayers.

Early Science Program Intrepid Allocation:
7.5 Million Hours

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Biological Sciences

How Do Researchers Predict the Structures of Biologically Important Proteins?

Proteins are the workhorse molecules of all biological systems. A deep and predictive understanding of life thus requires a detailed picture of their structure. Conventional protein structure determination using nuclear magnetic resonance (NMR) relies primarily on side-chain proton-proton distances. The necessary side-chain chemical shift assignment, however, is expensive and time-consuming, with possibilities for error. Moreover, approaches to NMR structure determination for larger proteins usually rely on extensive deuteration, which results in loss of key proton-proton distance information. Sparse structural data can be obtained from backbone-only experiments like orientational restraints from residual dipolar couplings and amid proton distances from NOESY spectra. These experiments are readily applicable even to fully deuterated and large proteins.

To determine NMR structures without side-chain chemical shift information, researchers incorporate backbone chemical shifts, residual dipolar couplings, and amide proton distances into the Rosetta high-resolution modeling methodology. To exploit the weak guidance signal provided by the sparse constraints, they developed an iterative scheme similar to a genetic optimization algorithm. A pool of the fittest individuals (e.g., lowest energy conformations) is maintained, and its worst part is replaced with offspring. The breeding or crossover of highly fit species (e.g., low energy conformations) is implemented as a Monte Carlo optimization that recombines features of previously found low-energy conformations. The type of features selected for recombination is adapted to the resolution of the pooled low-energy structures.

The iterative protocol increased the size range of accessible protein structures compared to the conventional Rosetta protocol. Researchers consistently solve protein structures up to 200 residues. Currently, they are determining the size range of this method and are testing further improvements. The INCITE program has been and will continue to be invaluable in its development.

Our INCITE work is focused on three areas currently. The first area is computing protein structures from very limited experimental data. With the INCITE computing resources, we are optimistic about developing methods which allow determination of the structures of proteins over 200 amino acids by NMR, which would be a big breakthrough in this area. The second area is designing proteins to bind very tightly to specific regions on a specified target. The third area is design of new enzyme catalysts. We are exploring catalysts for hydrogen production, solar capture, and other energy-related applications.

INCITE Allocation:

50 Million Hours

"The INCITE program continues to be invaluable in our research."

Researchers determined this large protein, ALG13, which is 200 amino acids in length, with a new methodology called "NMR structure determination without side-chain assignments."

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Biological Sciences

Modeling the Molecular Basis of Parkinson's Disease

As the second most common neurological disorder in adults, the personal and economic impacts of Parkinson's disease are enormous. Currently, there are more than 2 million cases in the United States. In economic terms, the disease exacts an annual cost of $25 billion on the U.S. economy alone.

University of California—San Diego scientists have shown that the aggregation of a protein known as alpha-synuclein (aS) in the brain can lead to harmful, pore-like structures in human membranes. Researchers are leveraging the high-end computation power of the Blue Gene/P at the Argonne Leadership Computing Facility (ALCF) to learn more about the molecular basis of the disease and to explore ways to treat it. Scientists used alpha-synuclein in specific conformations as templates for possible pharmacophore hypotheses design. Such an approach made possible the design of drug candidates for the cure of Parkinson's disease.

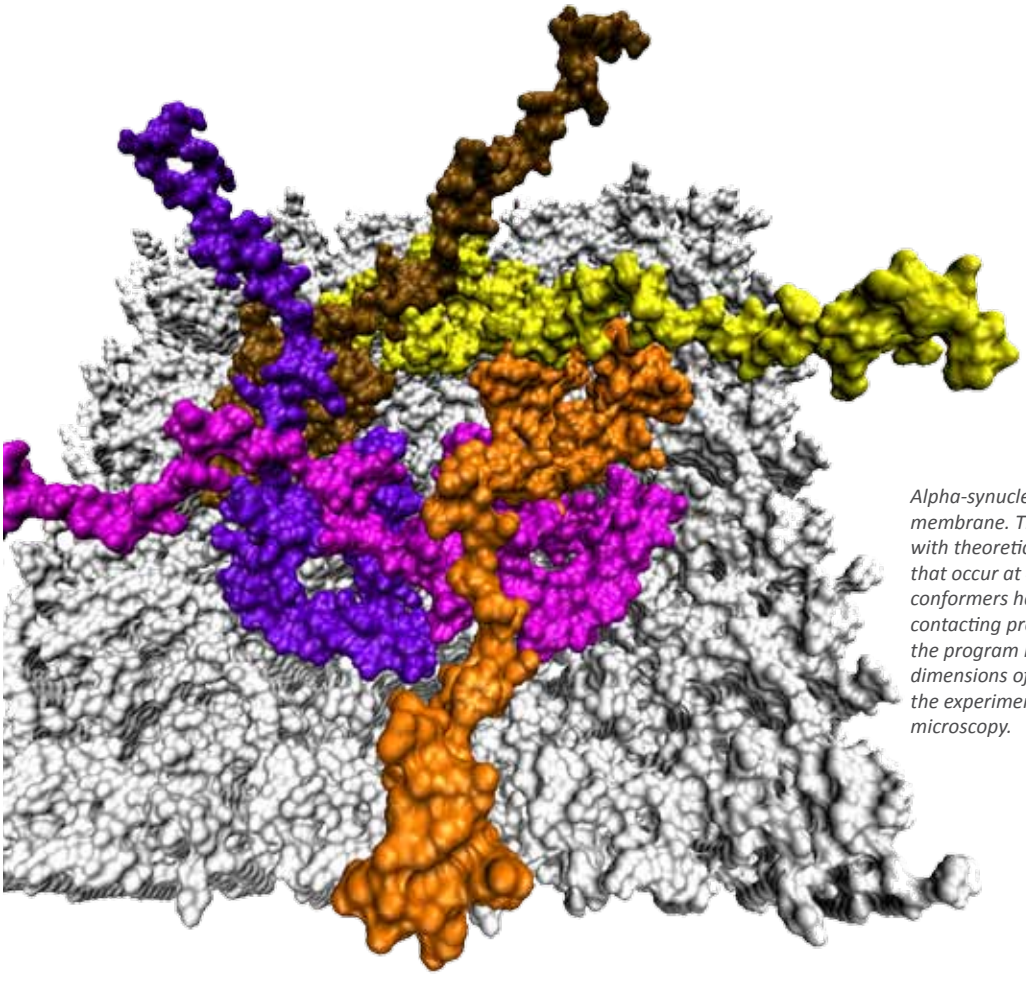
Research is providing insights into the molecular mechanism for Parkinson's disease progression and will have broad applicability to other diseases. The findings also provide a test bed for identifying possible therapeutic interventions through computational modeling.

Collaborator Dr. Eliezer Masliah and his laboratory are conducting experimental validation of the modeling and simulation results obtained. Given the encouraging correlation between the computational modeling predictions and laboratory experimental results, the team expects to make steady progress both with the computational model itself and with the design of effective drugs based on the computational modeling and simulations.

The research team will focus on a more comprehensive investigation of alpha-synuclein penetration into the membrane, including a thorough study of pore creation. The scope of the team's work has increased in both the number of simulations being conducted and the scale of the simulations.

INCITE Allocation:

5 Million Hours



Alpha-synuclein pentamer on the membrane. The pentamer is constructed with theoretical docking of Asyn conformers that occur at 4 ns of MD simulation. These conformers have the best membrane contacting properties (calculated by the program MAPAS). The geometrical dimensions of this pentamer correspond to the experimentally elucidated by electron microscopy.

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Biology

Multiscale Molecular Simulations at the Petascale

Early Science Program
Intrepid Allocation:
7.5 Million Hours

Project results will directly impact the understanding of cellular-scale biological processes via coupling of multiscale computer simulation methodology with petascale computational algorithms and hardware. When combined with leading-edge experimental research, the project will provide key scientific advances relevant to human health and the understanding of the biological world.

Researchers will apply multiscale bio-simulation methodology to three scientific problems: (1) Simulation of key steps of the HIV viral replication cycle. The human immunodeficiency virus type 1 (HIV-1) begins assembly with multimerization of the Gag polyprotein near the plasma membrane of infected cells. There has been debate over exactly how many Gags are in the immature virion. The researchers will use their methodology to construct coarse-grained (CG) models directly from structural biology experiments and physics-based interaction modeling. (2) Simulation of the Ribosome. Protein biosynthesis is a core life process in cells, which is mainly achieved by ribosomes. Since the ribosomes are targets for drugs such as antibiotics, a deep understanding of the mechanism of protein synthesis can aid in drug discovery. (3) Simulation of microtubules. Microtubules are one of the key components of the cytoskeleton, involved in trafficking, structural support, and cytokinesis. Microtubules are polymers assembled from alpha/beta tubulin dimers in the form of tubes with a diameter of 25 nm and variable lengths. Because of their size and the long timescale dynamics of these assemblies, these large and important protein assemblies inherently require a petascale multiscale simulation approach.

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Chemistry

Accurate Numerical Simulations of Chemical Phenomena Involved in Energy Production and Storage with MADNESS and MPQC

Researchers propose to focus on the problems of catalysis and heavy element chemistry for fuel reprocessing—both of which are of immediate interest to the Department of Energy (DOE), are representative of a very broad class of problems in chemistry, and demand the enormous computational resources anticipated from the next generation of leadership computing facilities. Also common to both is the need for accurate electronic structure calculations of heavy elements in complex environments.

Early Science Program Intrepid Allocation:
7.5 Million Hours

Catalysis: A catalyst greatly improves the efficiency of a desired chemical reaction, and catalytic processes are directly involved in the synthesis of 20% of all industrial products. Within the DOE mission, catalysts feature prominently in cleaner and more efficient energy production, exemplified by the fuel cell and storage technologies. To date, catalysts have been designed largely using trial and error, e.g., synthesizing and testing a potential new catalyst to determine if the reaction is more efficient. This process is both expensive and time-consuming and rarely leads to novel catalysts. Computational modeling and simulation can improve this process, supporting experiment by improved analysis and interpretation of data, and ultimately, in partnership with experiment, enabling the design of catalysts from first principles. Researchers will focus, in collaboration with experimentalists at ORNL, on chemical processes on imperfect metal-oxide surfaces.

Heavy element chemistry for fuel reprocessing: In collaboration with experimentalists and theorists, researchers will focus on two aspects of heavy element chemistry for fuel reprocessing: molecular interfacial partitioning and ligand design. Critical to both are rapid, yet quantitative, models for the interaction of heavy elements with novel organic ligands, and the interaction of both with a multispecies solvent. Speed is essential for combinatorial design due to the evaluation of a huge number of candidates, and also to enable *ab initio* dynamics for the inclusion of finite temperature and entropy.

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Chemistry

High-Accuracy Predictions of the Bulk Properties of Water

Among the *ab initio* methods, second-order perturbation theory (MP2) predicts highly accurate structures and relative energies for water clusters. Researchers will carry out molecular dynamics simulations of water at the MP2 level. However, full MP2 calculations of even modest-sized water clusters are far too time-consuming for dynamical simulations, even on the next-generation Blue Gene. Therefore, a key element of the current approach will be the use of MP2 in conjunction with the Fragment Molecular Orbital (FMO) method. Compared with today's calculations, researchers will determine the bulk properties at higher levels of accuracy using larger basis sets, larger embedded clusters, and longer dynamics simulations, as permitted by the greater computational capacity available with the Blue Gene. They will target the following bulk properties of water: structure, density, refractive index, diffusion constant, free energy, heat capacity, dielectric constant, vaporization enthalpy, isothermal compressibility, and thermal expansion coefficients. The final eight properties are more difficult to obtain than the first two. While Blue Gene/P gives good estimates, the greater capacity of the next-generation Blue Gene will be critical to establishing convergence of these properties with respect to theory, basis set, cluster size, and simulation length. There have been conflicting reports in the literature about the relevance of "chain" or"ring" networks in water. The high-accuracy simulations on the next-generation Blue Gene will help settle this argument about the structure of liquid water.

Early Science Program
Intrepid Allocation:
2 Million Hours

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Chemistry

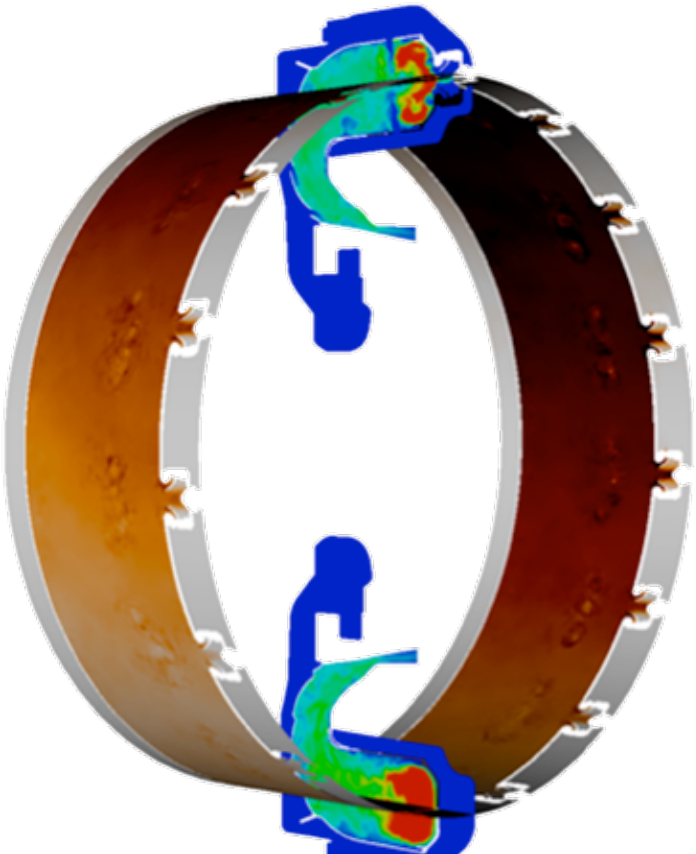
Performing the Largest Unstructured Large Eddy Simulation of a Real, Full Combustion Chamber

The increase of computer power has allowed science to make important strides in a variety of domains such as plasma studies, biomechanics, and molecular dynamics. With access to the INCITE program, researchers from CERFACS (the European Centre for Research and Advanced Training in Scientific Computation) have been able to perform top-of-the-line quality simulations on highly complex cases in their goal towards the fully numerical modeling of a real combustor.

This research is focused on Large Eddy Simulation (LES) of gas turbine engines with the inclusion of liquid phase phenomena. CERFACS has performed simulations and validation of two-phase flow experiments. In parallel, taking advantage of the leadership-class computer available at the Argonne Leadership Computing Facility, the researchers have performed the largest unstructured LES done to date of a real, full combustion chamber (330 million elements) on more than 16K cores. This simulation contributes to the validation of the LES approach when dealing with combustion instabilities. In these cases, the effects of mesh refinement are a highly critical point that was validated during the Stanford Center for Turbulence Research (CTR) summer program. A second mesh independency validation was performed, but this time it used a simpler, two-phase-flow single burner with three levels of refinement (4-, 8-, and 16-million elements). These results were published in the CTR Proceedings of the 2010 Summer Program by Cambridge University Press. Evaluation of the unbalance observed in Lagrangian simulations remains to be performed.

INCITE Allocation:
8 Million Hours

"The impact of the INCITE project on our research is essential because it brings capacities that were simply not available up to now and allows us to compute real engines and not only laboratory-simplified setups. The development of the solver itself in collaboration with Argonne research scientists is also essential. Our team has worked with the ALCF's Dr. Balakrishnan at Stanford this summer, finishing the 330-million-cell compressible simulation, which had never been done before. Together, we also have sent a proposal for the G8 exascale initiative, in which we prepare our codes for the next-generation machine."



Fields of temperature and pressure in a simulation of a complete helicopter combustion chamber performed on the IBM Blue Gene/P at the ALCF (July 2010).

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Chemistry

Predicting Bulk Properties of Water Systems

Ames Laboratory researchers are using high-quality electronic structure theory, statistical mechanical methods, and massively parallel computers to predict bulk properties of water systems that require high fidelity. This molecular-scale challenge is of critical importance to national scientific issues such as global warming and the environment.

The research under way is targeting very large systems whose sizes can only be addressed with massive computational resources. The researchers are using GAMESS and NWChem codes in simulations on Intrepid, the IBM Blue Gene/P housed at the Argonne Leadership Computing Facility (ALCF). Both codes are without question the two most broadly distributed scalable electronic structure systems. The research is focused on understanding the molecular-level dynamics of water, the formation of aerosols important in cloud formation, and the interactions of dendrimers with ligands of environmental importance. In each of these applications, the underlying research is setting a new standard for the predictive computation of bulk properties.

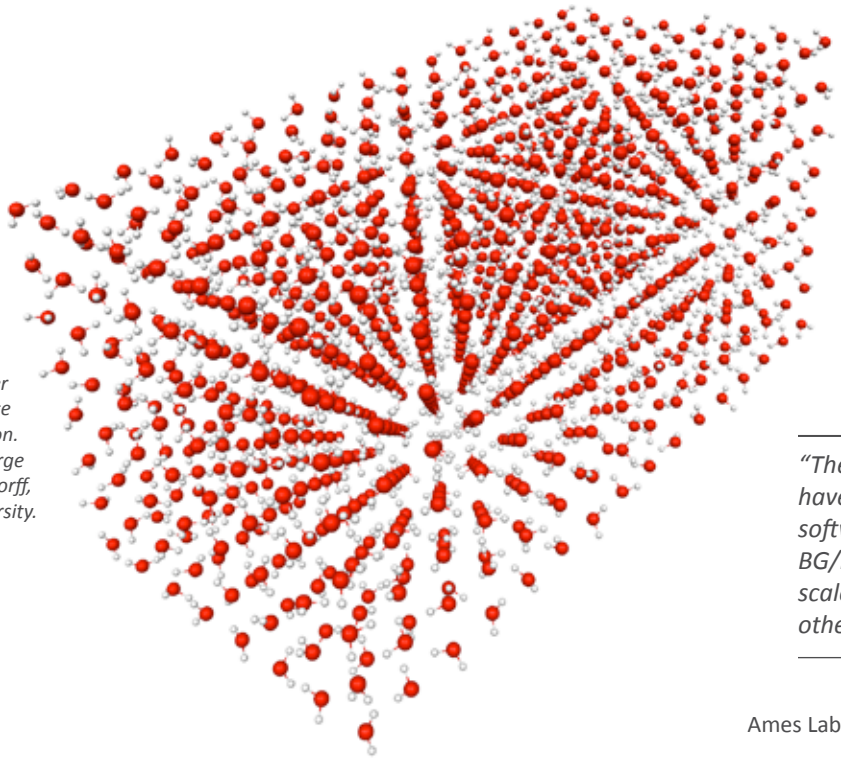
Large clusters of water are now amenable to molecular dynamics simulations with the large improvements that have been made in the Fragment Molecular Orbital (FMO) method in GAMESS. Graham Fletcher at the ALCF has been instrumental in making these improvements. As the results below show, 32 racks of the BG/P system can be very effectively used for these simulations.

INCITE Allocation:

8 Million Hours

		BG/P Racks:	1	2	4	8	16	32
		Cores:	4,096	8,192	16,384	32,768	65,536	131,072
Waters	Atoms	Basis Functions	Wall-time-to-solution (minutes)					
128	384	5504	8.6	4.8	2.7	1.8		
256	768	11,008	19.8	10.5	5.8	3.4	2.4	
512	1536	22,016		28.9	15.4	8.6	5.1	4.2
1024	3072	44,032			41.1	22.0	12.4	8.0

This research will impact a broad area of the chemical sciences and forge a path for subsequent research by the community.



1,024 water molecules in a lattice configuration. Credit: George Schoendorff, Iowa State University.

"The INCITE program and staff have allowed us to scale our software to 32 racks of the BG/P and to perform large-scale simulations that would not otherwise be possible."

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Chemistry

Simulation of Large Conformational Transitions in Macromolecular Systems Using Leadership Computing

Specialized strategies maximize simulation studies of protein gating

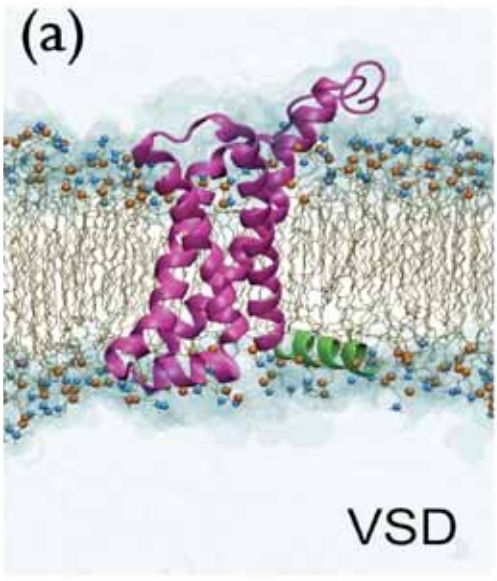
Atomistic molecular dynamics (MD) simulations are increasingly helping us to understand complex macromolecular systems. It is, however, essential to develop special strategies to get quantitatively meaningful results that can be compared with experiments. Many questions cannot be addressed with "brute force" MD simulation methods. Special methods and strategies are needed, for example, to treat large-scale motions in macromolecules to best use leadership-computing resources such as Argonne's Blue Gene/P.

Novel approaches field tested on Intrepid

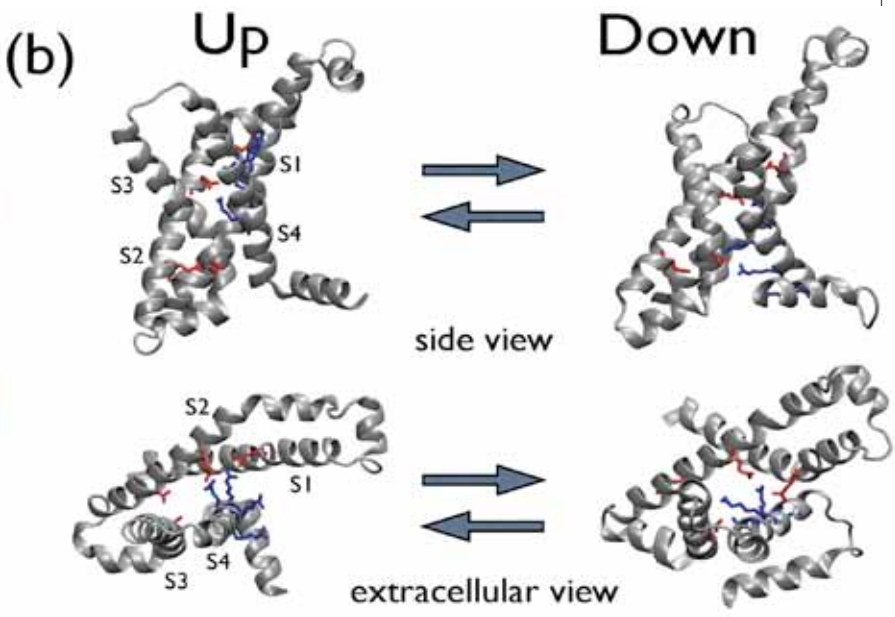
In this project, researchers will develop novel and cutting-edge approaches based on the string method with swarms-of-trajectories and Milestoning with Voronoi tessellation for characterizing large conformational transitions in complex macromolecular systems. They will use Intrepid to compute the transition pathway for the activation of the voltage-gated Kv1.2 potassium channel, a membrane-associated protein that functions as a molecular switch. This will be the first "field testing" of this novel and advanced methodology on a large macromolecular system.

ALCC Allocation:

28.5 Million Hours



(a) A snapshot of the atomic model of the isolated Kv1.2 VSD in the active (up) configuration from MD simulations in explicit water-membrane environment



(b) End-states of the VSD conformational transition for the VSD, from MD simulations: top row, side view; bottom row, extracellular view; positively charged residues on helix S4 are colored in blue, while acidic residues on helices S1, S2 and S3 are in red.

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Climate Research

Assessing Future Hurricane Impacts

Researchers at the National Center for Atmospheric Research (NCAR) and the Argonne Leadership Computing Facility (ALCF) are using the Nested Regional Climate Model (NRCM) on the ALCF's Blue Gene/P to develop improved assessments of impacts from Atlantic hurricanes over the next several decades.

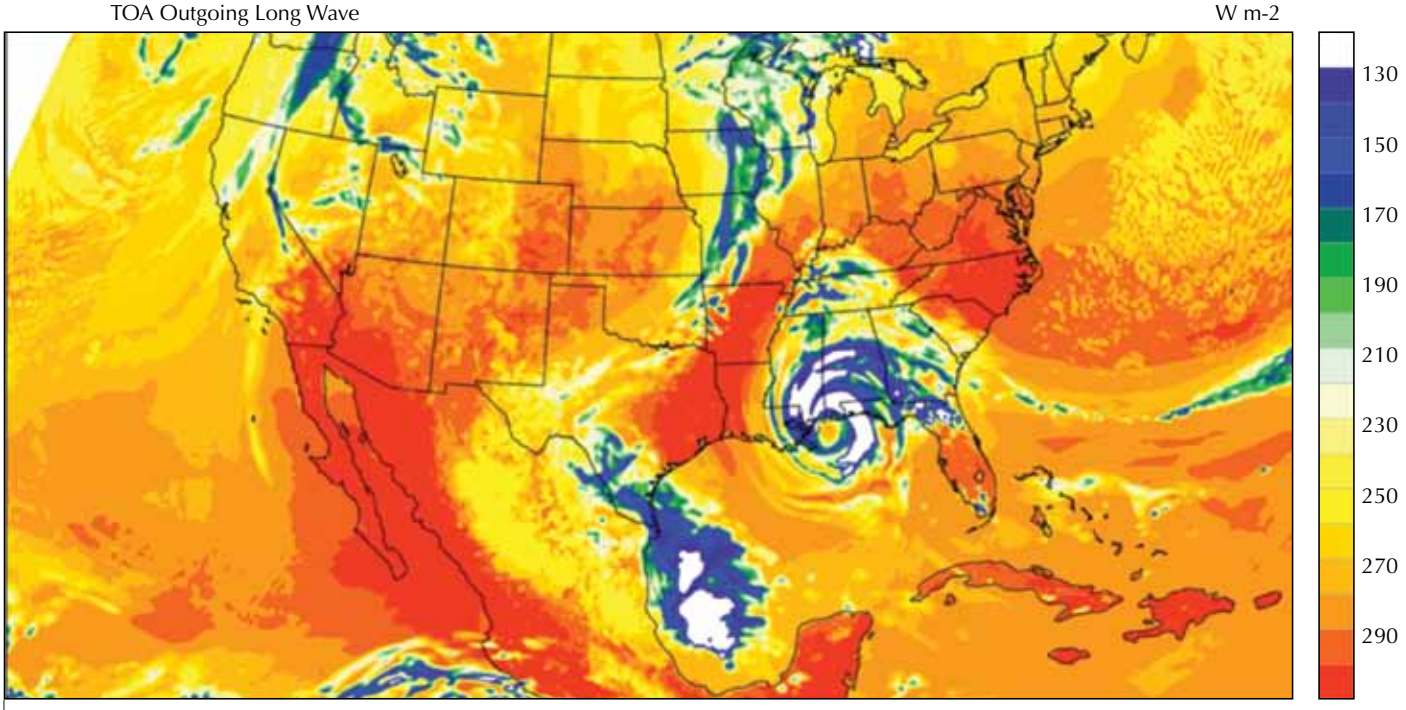
The NRCM combines the widely used Weather Research and Forecasting (WRF) model and the Community Climate System Model (CCSM). Through this combination, NRCM is able to effectively utilize both the climate simulation capacity of CCSM and the hurricane capacity of WRF to provide improved predictions of future hurricane activity to major societal and industry groups.

The work is contributing to a DOE-industry collaboration under the Research Partnership to Secure Energy for America (RPSEA) program, with emphasis on changing characteristics of hurricanes in the Gulf of Mexico offshore oil and gas fields. Research to date has indicated an increase in hurricane intensity through 2050. But this is countered by the hurricanes being smaller and faster, so that the net damage potential is predicted to decrease slightly.

Director's Discretionary Allocation:

17 Million Hours

"By using the ALCF facility, the NRCM is able to conduct the simulations at a very high resolution (equivalent to today's hurricane forecast models) so that critical details of hurricane formation, structure, and intensity can be simulated. This will further improve the prediction of hurricane impacts on our critical offshore energy infrastructure."



A Category 3 hurricane, making landfall along the Gulf Coast in October 2047, generated by the Nested Regional Climate Model.

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Climate Research

Climate-Weather Modeling Studies Using a Prototype Global Cloud-System Resolving Model

Scientists expect the understanding of the role of clouds in climate to undergo a qualitative change as the resolutions of global models begin to encompass clouds. At these resolutions, non-hydrostatic dynamics become significant and deep convective processes are resolved. Scientists are poised at the threshold of being able to run global scale simulations that include direct, non-parameterized, simulations of deep convective clouds.

The goal of this project is to use the next-generation Blue Gene system to explore the frontier of weather prediction and climate modeling with the newly developed Geophysical Fluid Dynamics Laboratory (GFDL) global cloud-resolving model. A single, unified atmospheric modeling system with a cubed-sphere dynamical core and bulk cloud microphysics running at hydrostatic (~ 10 km) and non-hydrostatic (<= 5 km) resolutions will be run with the goal of capturing the climatology of clouds and severe storms in a warming world. The ability to reproduce historical tropical storm statistics will be used as a test of this ground-breaking model. The purpose of the experiments proposed is to validate the global cloud-resolving climate model via hurricane hindcasts. For this purpose, the scientists will perform hurricane verification studies for the 2008 Atlantic Season. Storms in 2008 lasted a total of 100 days; performing 5-day forecasts on each of the days would give a total of 500 forecast days for the season.

Early Science Program Intrepid Allocation:
7.5 Million Hours

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Combustion

Direct Numerical Simulation of Autoignition in a Jet in a Cross-Flow Combustion

Lean combustion turbines provide excellent opportunities for environmentally friendly propulsion and electricity generation, but are severely limited by the danger of autoignition of the fuel-air mixture before its proper location. Further development of next-generation devices hinges upon better understanding of autoignition in flows that are characterized by considerable fluctuations of velocity, composition, and temperature. The aim of this project is to study the fundamental aspects of autoignition in a fuel-air mixing pattern directly applicable to mixing ducts in gas turbines. The Nek5000-based combustion code will be used to perform very large-scale direct numerical simulations of autoignition of a diluted hydrogen jet in a cross-flow of hot turbulent air in a laboratory-scale configuration. Detailed description of chemistry and molecular transport will be used to investigate the flow and scalar fields under cold and reactive conditions. It will also be used to construct databases that will be explored for years by engineers and scientists working in engine development for the construction and validation of advanced combustion models for engineering-type computational fluid dynamics codes.

Early Science Program
Intrepid Allocation:
5 Million Hours

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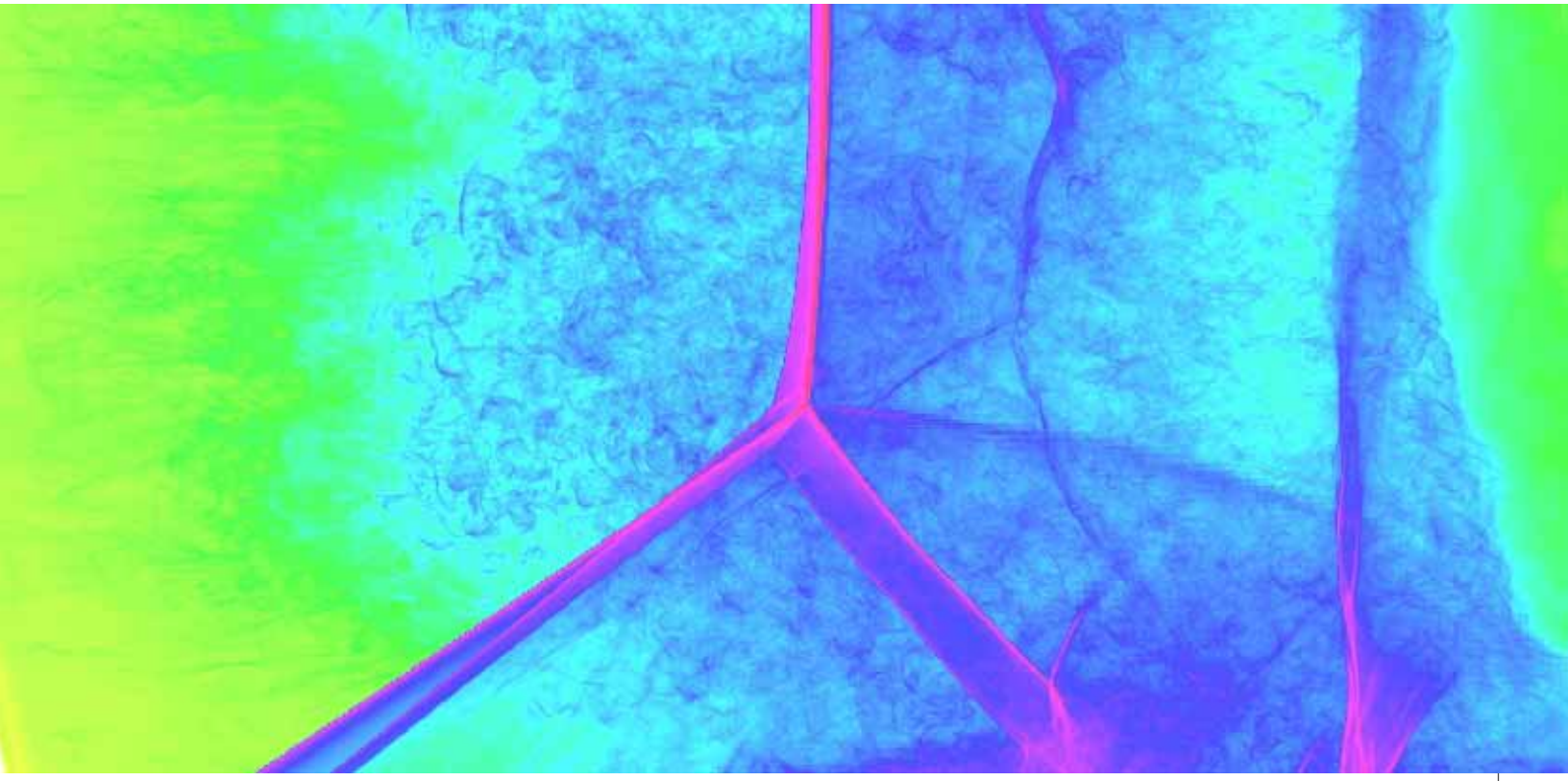
Combustion

High-Speed Combustion and Detonation (HSCD)

This project will gain insight into the physical mechanisms of the burning and detonation of hydrogen-oxygen mixtures. It will produce simulations to be used for the design of safe systems for future use of hydrogen fuel. The goal of the project is to create first-principles, petascale direct numerical simulation tools for understanding and predicting high-speed combustion and detonation (HSCD) phenomena in reactive gases. Researchers want to use first-principles simulations for fundamental understanding of the complex multi-scale physics of the transitory regimes of rapid flame acceleration and deflagration-to-detonation transition (DDT). The next-generation IBM Blue Gene system will enable them to perform first-principles simulations of DDT in a stoichiometric 2H2 + O2 mixture initially at atmospheric pressure in a 100 × 2.5 × 2.5 cm square tube. This is similar to a typical setup of the DDT experiments that measure run distances to detonation in reactive gases. Run distance is a critical parameter used for characterizing sensitivity of a reactive mixture to DDT, and it is used for assessing detonation hazard and designing severe accident mitigation strategies. In the experiments, burning is initiated by igniting a laminar flame in a quiescent gas near the closed end of the tube. As the flame expands, the turbulent boundary layer that forms near the tube walls increases the burning rate, and the flame accelerates rapidly. Secondary shocks and pressure waves generated inside the flame brush add to flame acceleration. Eventually this leads to a localized explosion and the onset of a detonation wave.

Early Science Program Intrepid Allocation:

5 Million Hours



Three-dimensional Navier-Stokes first-principles direct numerical simulation of a Mach=3 reflected shock bifurcation in a hydrogen-oxygen mixture in a square channel, performed within the high-speed combustion and detonation project (HSCD). Pseudo-schlieren image of a temperature field. Credits: Alexei Khokhlov (U of C), Charles Bacon (ANL), Shashi Aithal (ANL), Joanna Austin (UIUC).

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The University of Chicago | ajk@oddjob.uchicago.edu

Computer Science

Implementing the TotalView Debugger on the ALCF's Blue Gene/P

The TotalView debugger is a tool used in all computational sciences during application development. Work on the TotalView debugger on the IBM Blue Gene/P supercomputer at the Argonne Leadership Computing Facility (ALCF) encompasses several facets. The first step focuses on getting TotalView up and running with all the same features that were implemented on the Blue Gene/L (e.g., no thread or shared library support). The second step involves TotalView porting work to include thread and shared library support. The final step uses the machine for benchmarking TotalView on an ongoing basis.

As the first two steps progress, changes to the Blue Gene software stack may be needed. Currently, the minimum-version level needed is V1R1M2_500_2007, which should include an update made in December 2007 to remove the setuid restriction on the mpirun process running on the front end node.

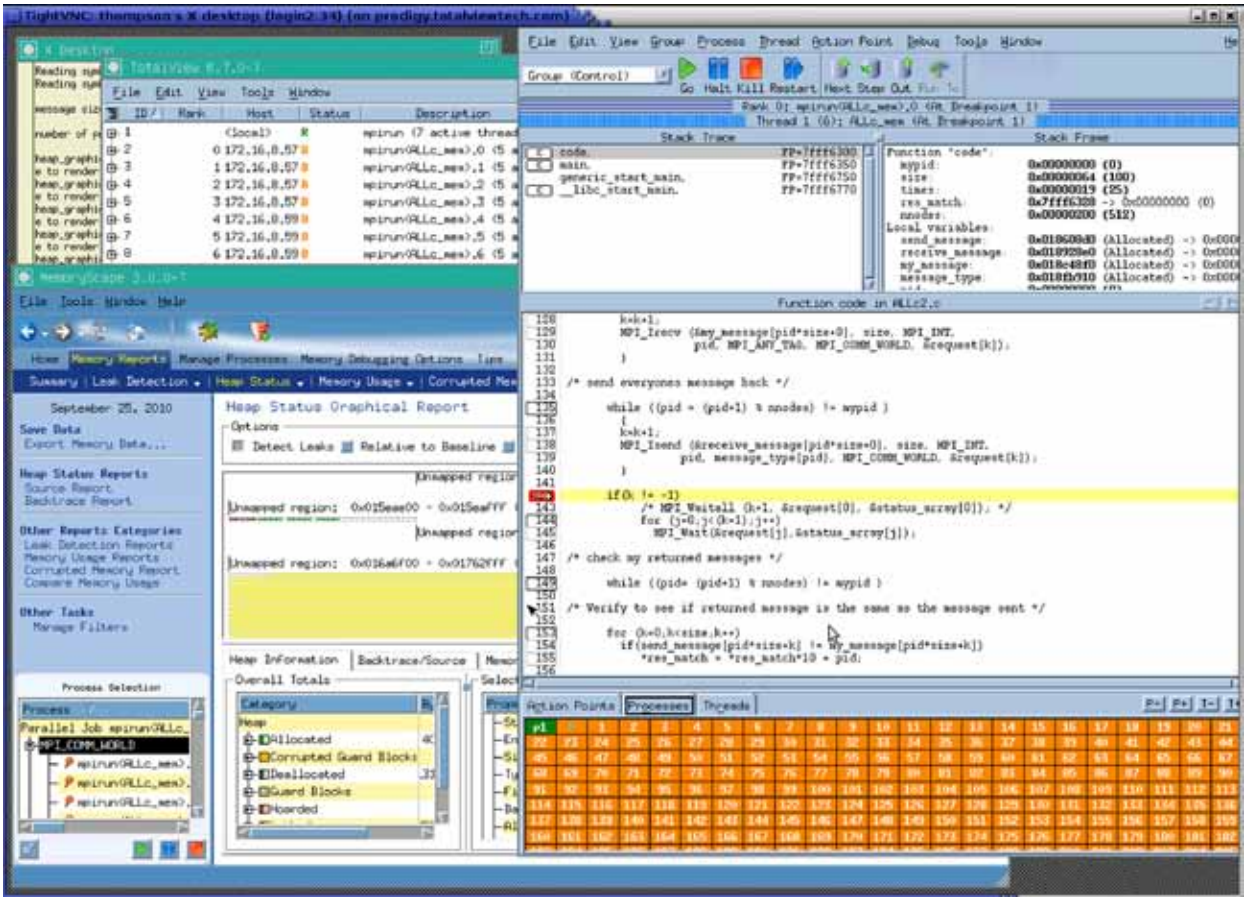
TotalView is currently working well on Blue Gene/P at driver level V1R4M2_200_2010-100508P. Threads and shared libraries are supported. Benchmarking work continues as we investigate performance.

The TotalView Debugger is a product of Rogue Wave Software. Developing parallel, data-intensive applications is hard. We make it easier.

Director's Discretionary Allocation:

5,000 Hours

"Any time gained working on the Blue Gene/P is welcome to us, as it will lead to better coding for our users."



TotalView screen shot.

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Computer Science

Repast SC++: A Platform for Large-scale Agent-based Modeling

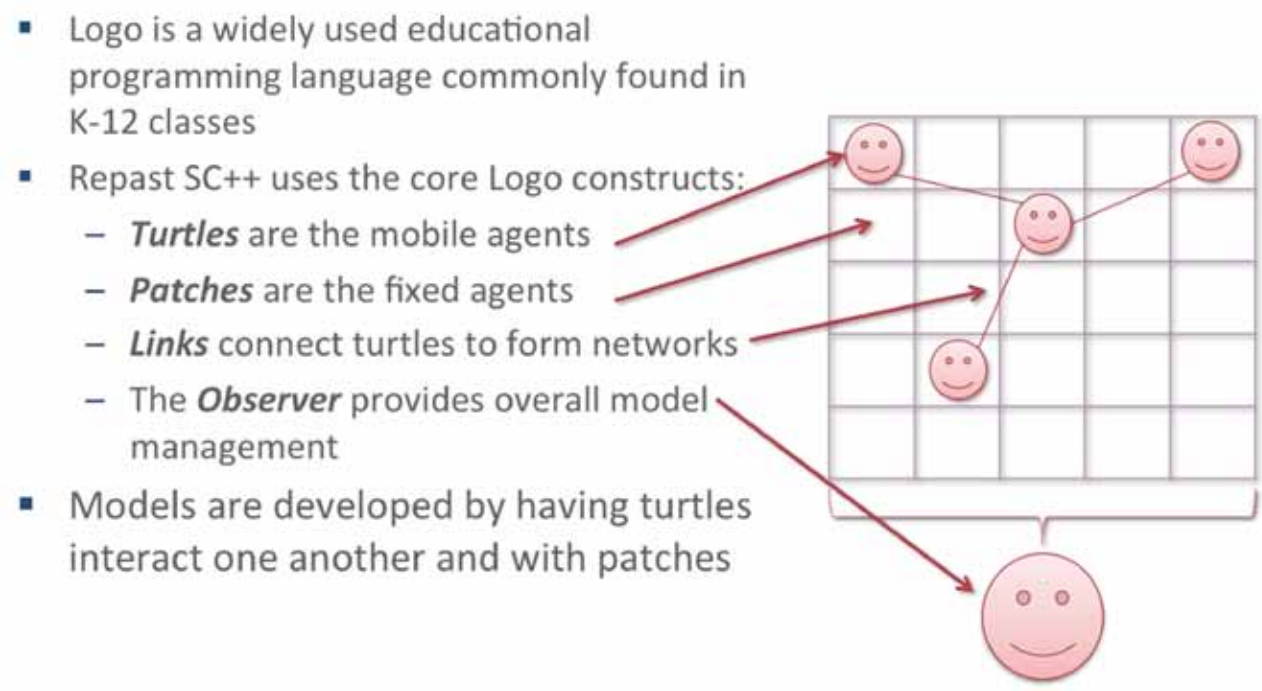
In the last decade, agent-based modeling and simulation (ABMS) has been successfully applied to a variety of domains, demonstrating the potential of this technique to advance science, engineering, and policy analysis. However, realizing the full potential of ABMS to find breakthrough research results requires far greater computing capability than is available through current ABMS tools. The Repast Simphony for C++ (Repast SC++) project addresses this need by developing a next- generation ABMS system explicitly focusing on larger-scale distributed computing platforms.

Repast SC++'s focus is on making possible distributed runs over many multiple processes. In doing so, Repast SC++ enables 1) massive individual runs – runs containing a number of agents sufficient to overwhelm a smaller number of processes; and 2) runs containing relatively few complex agents, where the computational complexity would overwhelm a smaller number of processes. Leveraging years of experience in ABMS toolkit and design and implementing the core Repast feature set, Repast SC++ is a useful and usable toolkit. It allows users to focus on model development and ignore the details of parallel programming. Written in portable C++, and using MPI and the boost libraries, Repast SC++ achieves "good enough" performance at large scales. Simulation models can be written in C++, using the core simulation components directly, or in a Logo-style C++ that uses the typical Logo turtle, patch, link, and observer components. (See figure below.) The Repast SC++ toolkit has been implemented and tested on the IBM Blue Gene/P at the Argonne Leadership Computing Facility. It will be released as an open source in October 2010. Repast SC++ is the subject of an invited chapter in the forthcoming book *Large-Scale Computing Techniques for Complex System Simulations.*

Director's Discretionary Allocation:

76,800 Hours

"This allocation has dramatically benefited our research by allowing us to test our platform at large scales."



Repast SC++ uses Logo to speed model development.

Contact ▸ **Michael J. North**
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Earth Science

A Proposal from the Geophysical Fluid Dynamics Laboratory to Perform Prototype Ultra High-Resolution Climate-Weather Modeling Studies at Argonne National Laboratory

ALCC Allocation:
25 Million Hours

Researchers will explore the frontier of weather predictions and climate modeling with the newly developed Geophysical Fluid Dynamics Laboratory (GFDL) global cloud-resolving model with bulk micro-physics. In addition to validating the model with test cases, they will conduct three types of numerical experiments: (1) global simulations to validate 5-day hurricane forecasts during one hurricane season, (2) high-resolution global simulations of selected hurricanes, and (3) longer-term climate simulations.

The name of the GFDL code they will use is HIRAM. As a preliminary, they will validate the model's stability and dynamical formulation by running the standard Held-Suarez test case.

First, the researchers will run a set of hurricane hindcasts. For each of the 100 days of the 2008 Atlantic hurricane season, they will run a 12 km (average grid resolution) global hydrostatic simulation for 5 simulated days to produce a 5-day forecast. They will compare these to actual weather data for those 5 days. For each run, they will initialize using actual historical data for the starting day.

Second, the researchers will run ultra-high resolution 4.5 km non-hydrostatic simulations on five selected storms. They will focus on accuracy of hurricane track and intensity predictions.

Third, the researchers will run one-year high-resolution 12 km global simulations of the year 2008. This will be an ensemble of five Atmospheric Model Intercomparison Project (AMIP) style runs. They will document the simulated climate and severe weather events (such as hurricanes and typhoons) during this period.

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Earth Science

How Can More Intricate Climate Models Help Curb Global Warming?

The effects of climate change are apparent in degrading air quality, intensified tropical storms, and the resulting destruction of coral reefs that protect the coasts from erosion and destructive waves. Global warming increases the occurrence of droughts, heat waves, wildfires, and floods. Scientists must improve the understanding of the impact of global warming so that society can optimally address climate adaptation considerations.

Advanced computation, like that possible on the Blue Gene/P at the Argonne Leadership Computing Facility (ALCF), allows researchers at the DOE laboratories and National Center for Atmospheric Research (NCAR) to develop more complex and intricate climate models. The vital information these improved models provide will help guide environmental policy.

The Department of Energy awards allocations of computing resources for climate studies across multiple laboratories through the INCITE program. In turn, the Climate Science Computational End Station (CCES) organizes and coordinates these computational efforts.

Using ALCF resources, CCES is advancing climate science through both aggressive model development activity and an extensive suite of climate simulations to correctly simulate the global carbon cycle and its feedback to the climate system, including its variability and modulation by ocean and land ecosystems.

Researchers are testing a new, highly scalable method for solving the fluid dynamics of the atmosphere for use in future climate simulations. This model, called HOMME, has run with a resolution as high as 1/8th of a degree of latitude on more than 80,000 cores.

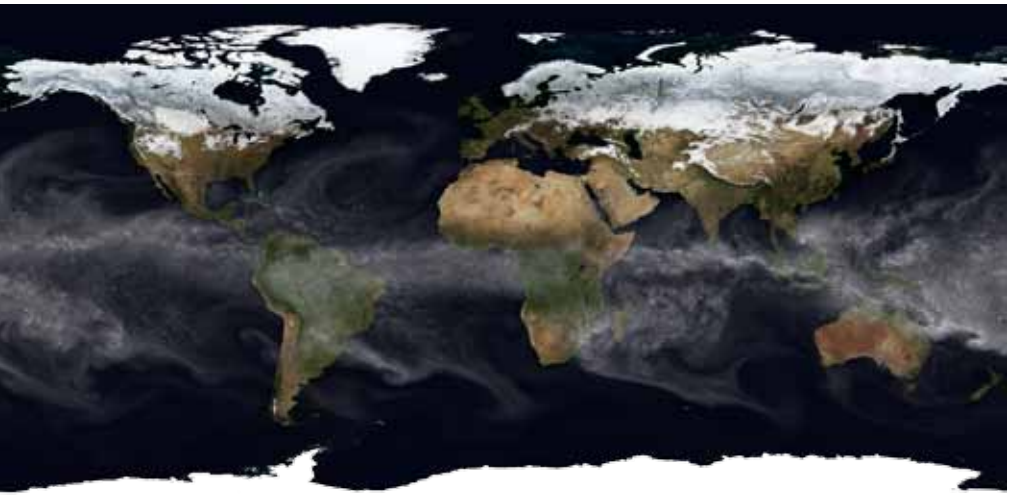
Next, researchers will use HOMME to perform standard climate model benchmark simulations for comparisons with other models. They will also test the new version of the Community Earth System Model on the ALCF's Blue Gene/P.

INCITE Allocation:

30 Million Hours

"As climate models evolve into fully integrated and realistic earth system models, the complexity of the simulations becomes enormous. Modeling the climate at these levels of complexity in a timely fashion requires massively parallel machines for fine-scale computational grids and expensive biogeochemistry and atmospheric chemistry packages. It is simply not possible without the opportunity afforded by the INCITE program."

--Tom Bettge, Coordinator for the CCES



Total precipitable water, a measure of how much moisture is in the air from a single moment in time in the global simulation of the atmosphere at a resolution of half a degree of latitude. (Figure provided by Mark Taylor, Sandia National Laboratories.)

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National Center for Atmospheric Research | wmw@ucar.edu

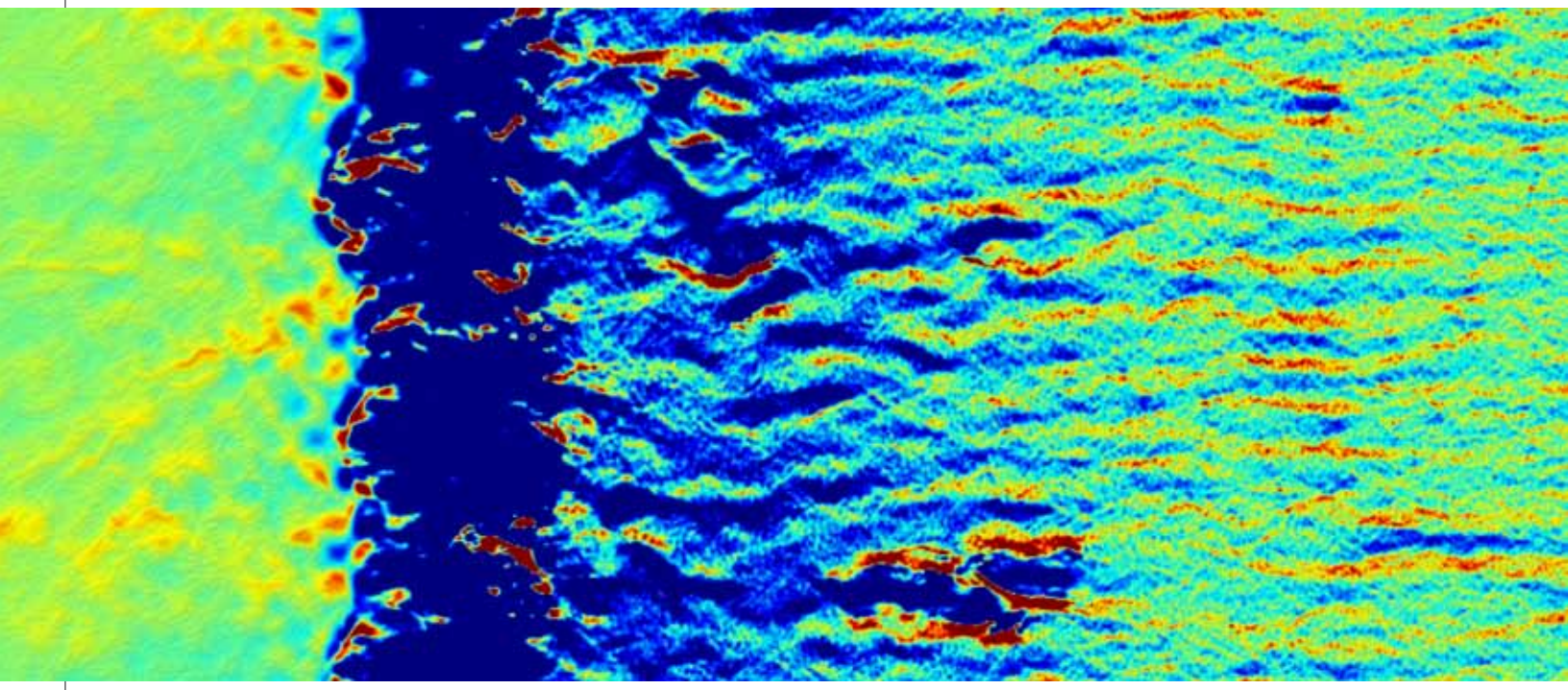
Energy Technologies

Exploring Particle-in-Cell/Hybrid Simulations of Fast Ignition

Fusion energy is one possible long-term energy solution that is both safe and environmentally friendly. Fast ignition is an alternative to conventional inertial confinement fusion currently pursued at the National Ignition Facility. This scheme separates the compression and heating phases from ignition, much like a petrol combustion engine. In the petrol engine, the fuel is compressed by the piston, and then ignited via the spark plug. In fast ignition, the driving lasers are the pistons, compressing the fuel to high density; then a second laser's high-intensity pulse serves as the "spark." Researchers from the University of California–Los Angeles (UCLA) have implemented a newly invented particle-in-cell (PIC)/magnetohydrodynamics (MHD) hybrid method that is 300 to 30,000 times faster than full PIC. The group is running three hybrid simulations of fast ignition targets, plus some full PIC/transport runs on Intrepid, the powerful Blue Gene/P supercomputer at the Argonne Leadership Computing Facility (ALCF).

INCITE Allocation:
7 Million Hours

Researchers from the University of California–Los Angeles (UCLA) have implemented a newly invented particle-in-cell (PIC)/ magnetohydrodynamics (MHD) hybrid method that is 300 to 30,000 times faster than full PIC.



Longitudinal electron currents of a fast ignition target irradiated by an ultrahigh intensity laser. As the laser hits the target front from the left-hand side, it generates a strong inward flow of electrons (blue) that is quickly compensated by a strong return current that builds up inside the target (yellow/red), leading to filamentation. Image generated from a simulation of the PIC code OSIRIS; Luís Silva, IST, Portugal; Warren Mori, UCLA.

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Energy Technologies

Improving Light Water Reactor Fuel Reliability Via Flow-Induced Vibration Simulations

Vibrations at the heart of fuel rod failures

Failures of the fuel rod elements used to power U.S. nuclear power plants are rare. When they do fail, however, one of the most common causes is flow-induced vibration of fuel assembly components. In fact, the Electric Power Research Institute reports that more than 70 percent of all fuel failures in pressured water reactors are due to grid-to-rod fretting.

Recent advances and state-of-the-art resources set stage for success

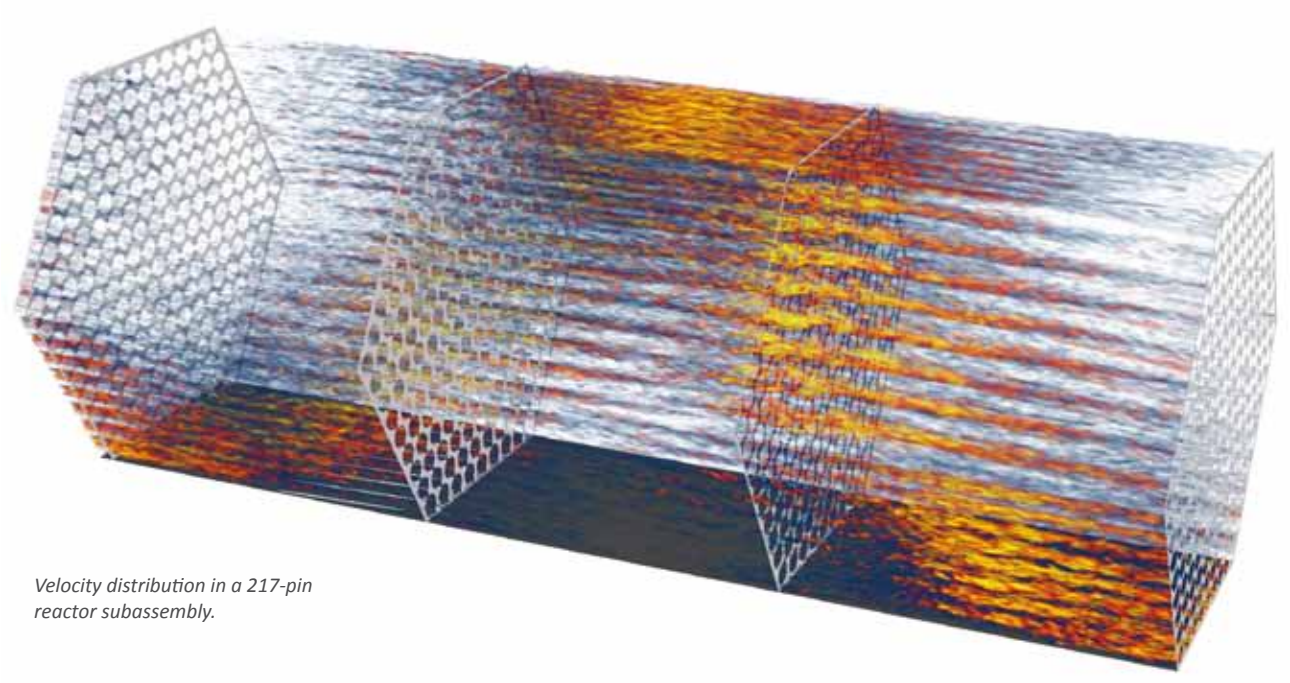
Using resources at the Argonne Leadership Computing Facility, scientists are investigating vibrations caused by turbulent flow in the core of light-water reactors—the major cause of fuel failure and a recognized bottleneck to optimal fuel utilization. This research is especially well timed, given recent advances in high-fidelity computational fluid dynamics that make multi-pin large-eddy simulations (LES) computationally within reach, coupled with fluid/structural codes that have reached a state of maturity far beyond what existed a decade ago.

Homegrown code, Nek5000, used to demystify forces in vibration

Researchers will conduct LES simulations using the Argonne-developed code Nek5000 to better understand vibration-driven forces resulting from the turbulent fluid flow in multi-pin configurations of realistic LWR fuel assembly geometries. These simulations will then be loosely coupled to the highly scalable finite-element structural mechanics simulator, Diablo.

ALCC Allocation:

75 Million Hours



Velocity distribution in a 217-pin reactor subassembly.

Contact ▸ **Andrew Siegel**
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Energy Technologies

Materials Design from First Principles

New materials may help solve global energy challenges

Our energy future hinges on the design and discovery of new materials—like materials to replace the oils currently used to make plastics and materials to power electric vehicles.

Scientists at Argonne's Center for Nanoscale Materials are pairing the power of the ALCF's Blue Gene/P with newly available electronic structure codes to conduct massively parallel quantum chemical calculations for use in the design of breakthrough materials that may have energy-related applications.

Materials reduce greenhouse gases, power electric vehicles

Research efforts will focus on catalytic materials and materials used for electric energy storage. Catalytic materials are used for bond-specific activation for efficient chemical transformations. This research could yield new strategies for more energy-efficient, environmentally friendly chemical synthesis to help reduce greenhouse gases, or in new methods for replacing petrochemicals with inexpensive, abundant small alkanes.

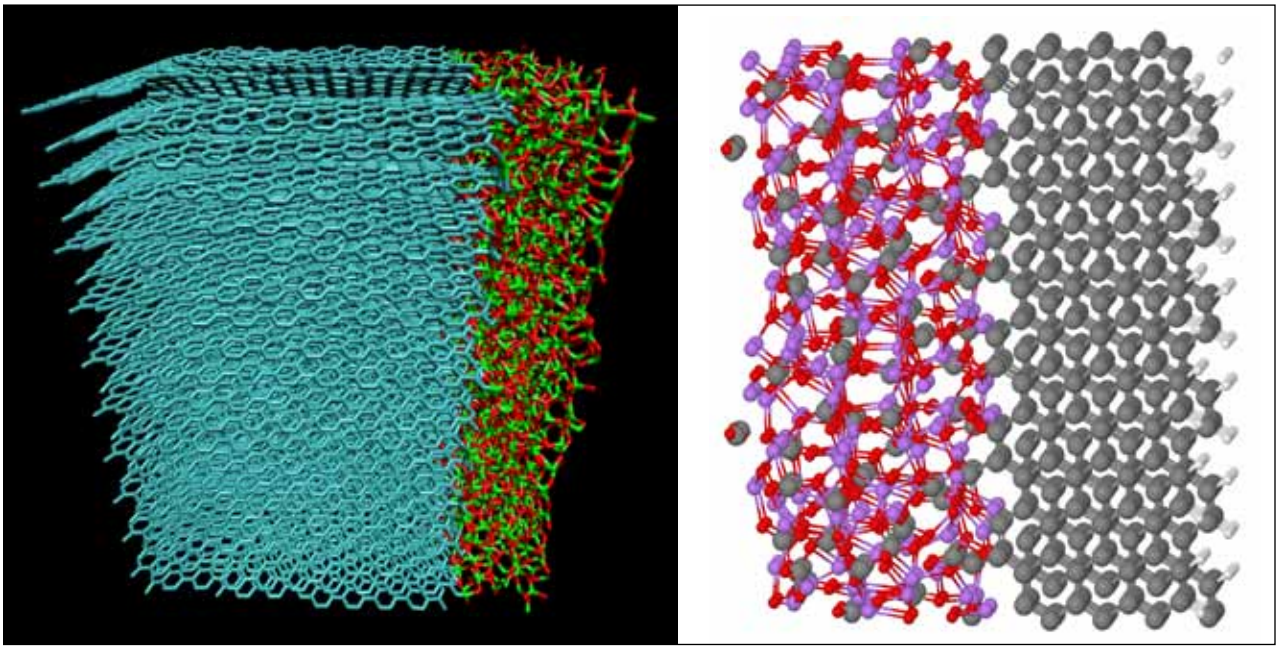
Creating new materials for electrical energy storage (specifically, for the interface between electrolyte and electrode) could lead to safer, longer-range batteries for electric vehicles.

Finding better solutions faster

With models of surfaces and interfaces in materials created from first-principles calculations not previously possible, scientists can conduct large-scale screening using a Materials Design Workbench developed at Argonne. Researchers will employ GPAW and NWCHEM codes adapted for massively parallel machines like the Blue Gene/P. Screening allows the scientists to focus efforts on the most promising materials.

ALCC Allocation:

20 Million Hours



Models for the solid electrolyte interphase in Li batteries: Amorphous alumina on graphite (left) and Li2CO3 on graphite (right).

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Energy Technologies

Petascale Direct Numerical Simulations of Turbulent Channel Flow

Researchers propose to use the petascale computing power of the next-generation Blue Gene system to perform direct numerical simulations (DNS) of high Reynolds number turbulent wall-bounded flow in a channel. This DNS is aimed at developing a nearly complete understanding of the phenomena dominating wall-bounded turbulence, which is central to the energy losses inherent in transportation. The impact of such a development will likely be profound. Approximately 28% of U.S. energy consumption is expended on transportation. This energy expenditure is due to the interaction between solid surfaces (of vehicles or pipes) and the fluid flowing past them, leading to drag and the dissipation of energy by turbulence. Since much of the drag in these flows is due to turbulent skin friction, much of this energy consumption results from wall-bounded turbulent shear layers.

The central emphasis of this research is on reaching a sufficiently high Reynolds number to explore the physics that arise in the overlap region. The overlap region is where the viscous near-wall turbulence interacts with the outer-layer turbulences. This interaction is key to understanding high Reynolds number turbulent wall layers. To investigate this interaction, it is necessary that the Reynolds number be sufficiently high so that there is a substantial disparity in scale between the inner and outer layers. The results can then be extrapolated to arbitrary Reynolds numbers. This simulation will be performed using the supercomputing software that the proposing team has developed and benchmarked on Blue Gene/P and will further optimize for performance on the next-generation Blue Gene.

Early Science Program
Intrepid Allocation:
5 Million Hours

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Energy Technologies

Scalable, Explicit Geometry, Whole-Core Nuclear Reactor Simulations

Multi-physics simulations aid design and safety in nuclear reactors

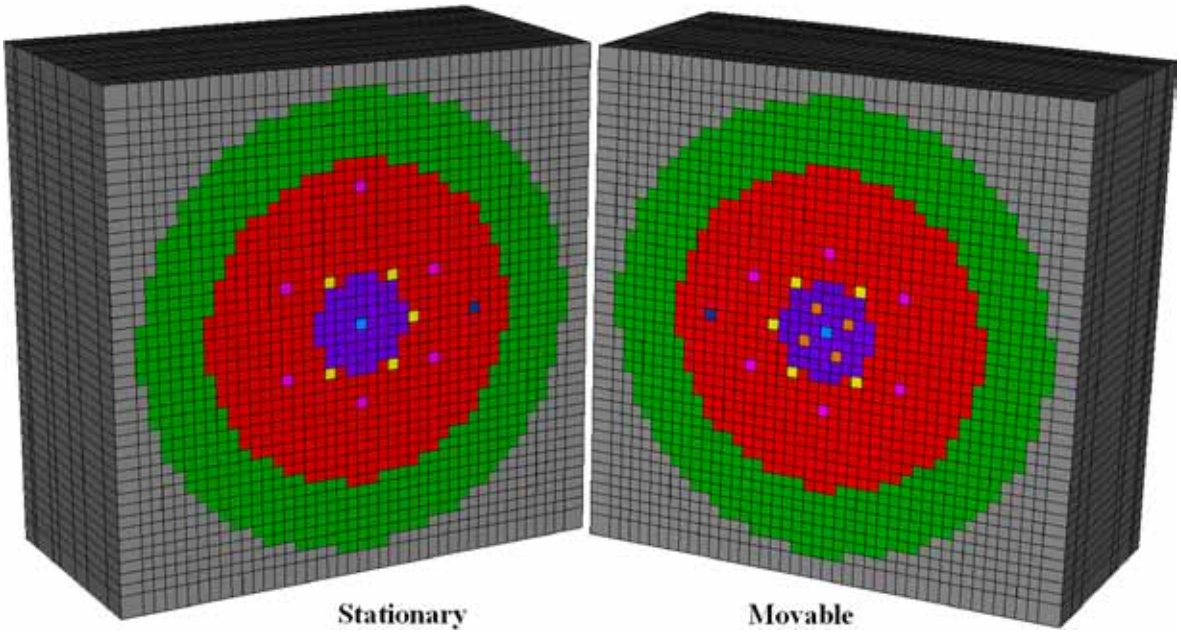
With its focus on solving nuclear energy issues, the Department of Energy is developing a multi-physics simulation framework at Argonne National Laboratory specifically for the analysis and design of nuclear reactors. Researchers will use this framework to simulate multi-physics problems requiring coupled neutronics, thermo-fluids and structural analyses. In such a framework UNIC can provide the power distribution on the deformed geometry, thereby allowing researchers to predict the change in power distribution derived from thermal expansion and improve the design and safe operation of nuclear reactors.

Full-scale simulation to validate high-performing UNIC neutronics code

UNIC has accurately predicted global parameters and has demonstrated excellent parallel computation performance for several benchmarking problems, including problems containing up to 0.9 trillion degrees of freedom and better than 75 percent weak scaling on the full capacity on the world's fastest and largest open science supercomputers. This work earned a finalist designation for the Gordon Bell Award at Supercomputing 2009. UNIC has also shown its capability to produce very detailed solutions, which first must be validated against experiments before it is fully coupled with thermo-fluid and structural analysis codes. For this validation, researchers will analyze the detailed reaction rate distributions measured in a full-scale critical experiment carried out in ZPR-6—the Zero Power Reactor facility at Argonne National Laboratory.

ALCC Allocation:

38 Million Hours



ZPR6/7 Loading 104 consists of a Pu filled core with a High Pu240 central core region. Loadings 104 through 132 focused on modifying the base case to study the impact of various material changes (sodium void, control rod worth, etc.). In loading 104, the fuel was removed from the center drawer to simulate a control rod position (control rod is not inserted) and foil measurements were carried out to investigate the altered energy dependence with respect to the other loadings.

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Argonne National Laboratory | masmith@anl.gov

Engineering

A Center for Turbulence Research - Argonne Leadership Computing Facility Collaboratory for Very Large Scale Turbulence Simulations on Petascale Computing Platforms

New turbulence collaboration enhances energy security

The Center for Turbulence Research (CTR) and the Argonne Leadership Computing Facility (ALCF) have joined forces to enhance the state of the art of turbulence simulations by harnessing the computing power of the Blue Gene/P via allocations from the ASCR Leadership Computing Challenge (ALCC) program.

The collaboration will focus on high-risk, high-payoff turbulence simulations linked to advancing national energy security, including studies of aerodynamic noise reduction in next-generation aircraft propulsion systems, heat transfer in advanced energy systems, and related simulations.

Reducing jet engine noise

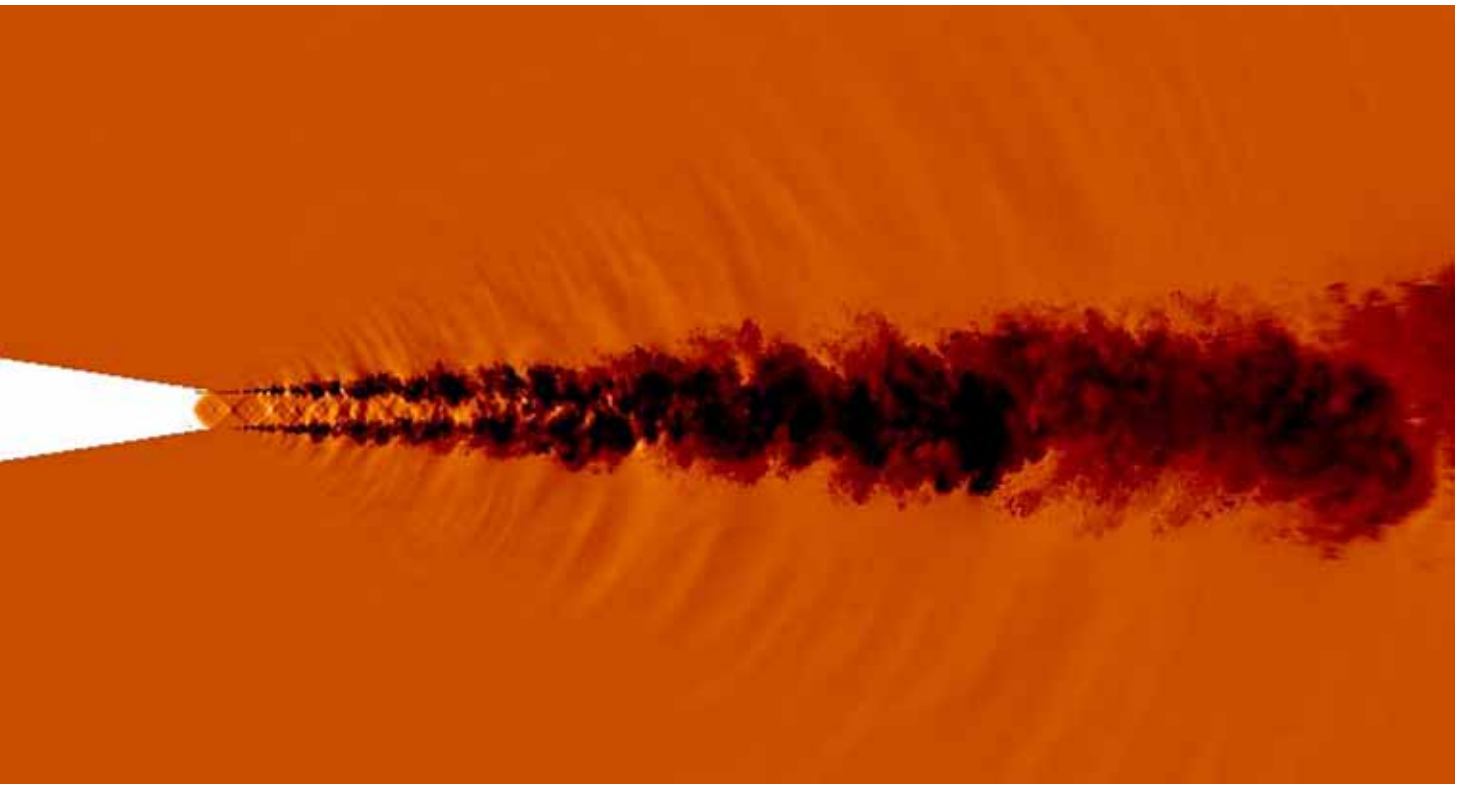
Initially, the CTR-ALCF collaboration will study the effects of chevrons on turbulent mixing of jet engine exhaust streams and on the role chevrons play in noise suppression. Chevrons—serrated geometric edges installed on aircraft engines—greatly reduce noise by mixing exhaust jet streams. Their design, however, must balance their role in reducing noise with performance reductions they might cause.

New simulations aim to tell the full story

To date, most simulations model the effects of chevrons by source-and-sink terms in the governing equations rather than by resolving their complex, small-scale geometric details. The proposed simulations aim to fully resolve the effects of the chevrons in a jet engine to capture the enhanced shear layer mixing the chevrons generate and, in turn, to evaluate possible noise-mitigation strategies.

ALCC Allocation:

50 Million Hours



Simulation of an expanding supersonic jet and the radiated acoustic field.

Contact ▸ **Parviz Moin**
Center for Turbulence Research, Stanford University | moin@stanford.edu

Engineering

Aerodynamics Exploration for Advanced Aero-Propulsion Technologies

The technologies targeted in this project are related to advanced propulsor design that employs low-pressure-ratio fan and its driving component, a lightweight, high-output low-pressure turbine. Advanced aero-engine propulsors employ higher bypass ratio, low-pressure ratio fan designs for improved fuel burn. Lower fan pressure ratios lead to increased propulsive efficiency, and besides enabling thermodynamic cycle changes for improved fuel efficiency, significant noise reduction can be achieved. However, as the fan pressure ratio and fan speed are reduced, the fan design becomes more sensitive to inlet flow distortion and installation stagnation pressure losses.

This project's effort focuses on the rigorous investigation of the underlying mechanism and the necessary technologies to reduce inlet distortion sensitivity and stability issues in low-pressure ratio aero-engine fan systems. The driving component for the propulsor, the low-pressure (LP) turbine strongly influences the specific fuel consumption of an engine, where a 1 percent increase in LP polytropic efficiency improves the fuel consumption by 0.5 to 1 percent. With efficiency levels already much greater than 90 percent, there will be little scope for improving this aspect of performance without a step change in technology. Increased-lift airfoils lead to reduction of number of airfoil needed for a specific stage loading level, hence the reduction of weight. Increased stage loading designs leads to higher power output or further weight reduction. Being able to understand and predict the unsteady transitional flow in LP turbines is essential in developing airfoils with increased lift and increased stage loading that retain the already high levels of efficiency. This represents an even greater challenge, especially as a reducing core size means that the Reynolds numbers are also reducing. The three-dimensional design of LP turbine airfoils also holds tremendous promise for achieving improved performance.

Researchers will use Department of Energy HPC resources at Argonne National Lab to explore the promising aerodynamic technologies that lead to the successful development of these aero-engine components, as these technologies require large-scale high-fidelity analytical capabilities. GE's in-house CFD code, TACOMA, will be used for these simulations. The numerical simulation is based on GE's turbomachinery flow software which solves time-unsteady Reynolds-averaged Navier-Stokes (URANS) equations. The underlying numerical algorithm leverages a parallel-efficient Jameson-Schmidt-Turkel (JST) Runge-Kutta scheme with dual-time stepping for unsteady flows. The software includes well-tested turbulence and transition models, as well as real-gas models and multi-phase flow capabilities.

ALCC Allocation:

4.5 Million Hours

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GE Global Research | yaoj@ge.com

Engineering

Delivering "Green" Low-Noise-Emission Wind Turbines and Jet Engines

Understanding the complex turbulent mixing noise sources for wind turbine airfoils and jet exhaust nozzles is critical to delivering the next generation of "green," low-noise wind turbines and jet engines. Scientists at GE Global Research are leveraging ALCF and the INCITE program to develop/prove hi-fidelity direct-from-first-principles predictions of noise to characterize these hard to measure acoustic sources.

A scalable, compressible Large Eddy Simulation (LES)–based Computational Aeroacoustics (CAA) solver is being used to study free-shear layer noise from jet exhaust nozzles and boundary layer noise sources from airfoils. Representative wind turbine airfoils have been simulated at realistic Reynolds & Mach numbers to mature CAA prediction accuracy. To prove design differentiation capability and hence readiness as a numerical rig ready to accelerate industrial design, the LES/large-scale HPC combination is being proven on a range of jet nozzle configurations. Fundamental scaling questions (Reynolds number) that bedevil testing are being answered. Significant improvement in the scalability of the solver on the BG/P platform to 32K cores also has been achieved.

Other results include:

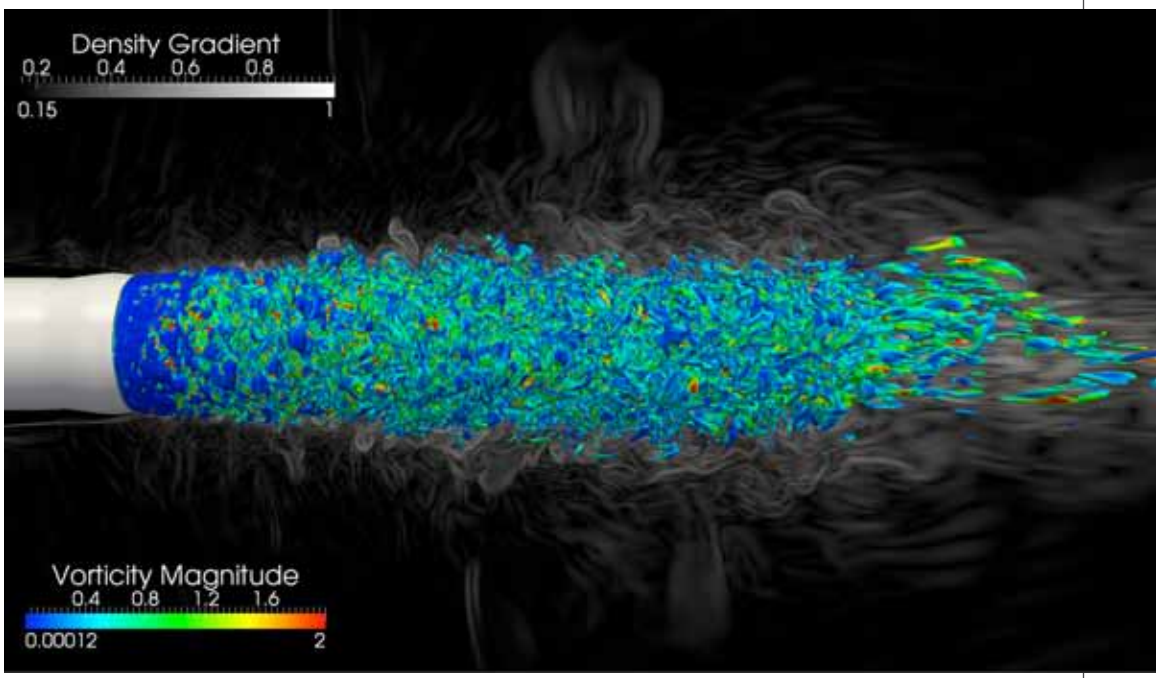
- Comparisons with experimental data show that the LES predictions for both single and dual-flow nozzles are successful in predicting the turbulent flow evolution. Far-field acoustics prediction based on the near field flow data compares very favorably to the experiments proving the ability of this first principles-based approach for design guidance.
- Preliminary investigation of the airfoil simulation demonstrates an ability to correctly predict the eddy convection velocity in the boundary layer – an important guide for improved source modeling

With proof-of concept aero and acoustic LES calculations completed, the team is pursuing the use of LES+HPC to:

- Design noise-reduction features,
- Demonstrate numerical wind tunnel capability,
- Improve efficiency of numerical algorithms and parallel scalability beyond 32K cores.

INCITE Allocation:

19 Million Hours



Turbulent structures in free shear layer flow from dual-flow conic nozzle– Vorticity contours plotted on constant Q surface.

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GE Global | guptaan@ge.com

Engineering

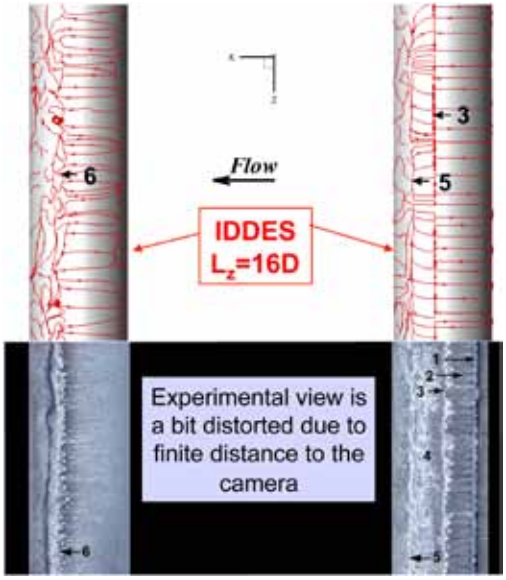
Employing Improved Delayed Detached Eddy Simulations for Turbulent Flows over Tandem Cylinders

The flow past Tandem Cylinders is a prime test case for detailed comparisons between CFD and experiments, with particular focus on the physics of massively separated flows, the impingement of turbulence on a solid body, and the noise that results from this interaction. Such flow scenarios occur in a wide variety of applications that include (but are not limited to) aircraft landing gear, wind turbines, bridges, industrial heat exchangers, and a myriad of architectural situations. Very recently, researchers from Boeing and NTS (St. Petersburg, Russia) have computed, on the IBM Blue Gene/P at the Argonne Leadership Computing Facility, massively separated flows over tandem cylinders using a novel algorithm known as the Delayed Detached Eddy Simulation (DDES) and its variant, the Improved Delayed Detached Eddy Simulation (IDDES). This new approach to computing turbulent flows creatively blends Reynolds Averaged Navier-Stokes (RANS) computations in the near wall region (i.e., at the surface of the cylinder) with Large Eddy Simulation (LES) computations in regions away from the wall. The tandem cylinder simulations on the Blue Gene/P are among the largest, with a computational domain spanning sixteen diameters in the cross-flow direction. Experiments done at NASA Langley indicate that at this span-wise length, the lateral pressure and velocity correlations begin to approach zero, thereby justifying the periodic boundary conditions used in the numerical simulations.

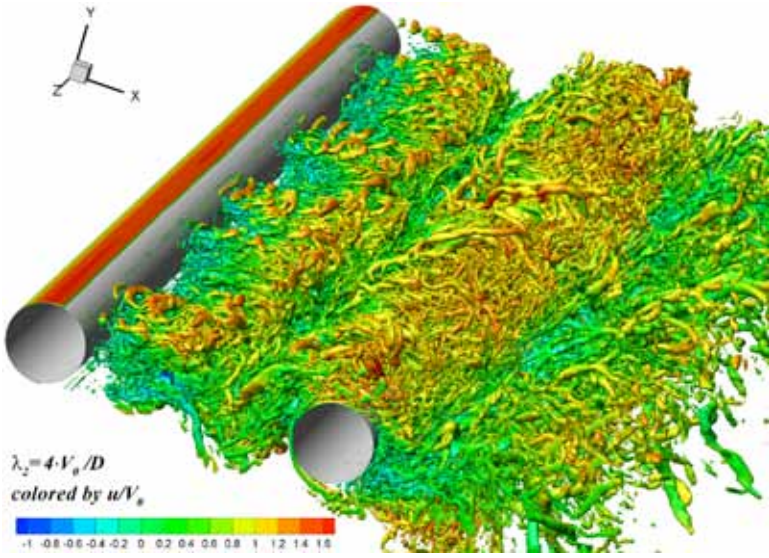
The NTS code, that has been used for the simulations, is a structured, multiblock, overlapping grid, finite volume code. The range of numerical schemes implemented in the code includes implicit high order hybrid (weighted 5th order upwind/4th order centered) flux difference splitting schemes of Rogers and Kwak for incompressible flows and of Roe for compressible flows. Numerical implementation of these schemes is performed by implicit relaxation algorithms (Plane/Line Gauss-Seidel relaxation and Diagonally Dominant ADI algorithm), which may be arbitrarily specified by a user in different grid-blocks. In addition, the code is capable of running in hybrid (i.e., MPI+OpenMP) mode and shows very good weak scaling on the Blue Gene/P.

Director's Discretionary Allocation:

11 Million Hours



Comparison of oil-flow patterns from DDES at Lz=16D with experiment: 1-transition strip; 2-streaks from streamwise vortices generated by transition strip; 3-primary separation line; 4-spanwise flow between 2 separation lines; 5-secondary separation line; 6-rear cylinder separation.



Isosurface of swirl λ=4.0V0/D for Lz=3D and Lz=16D

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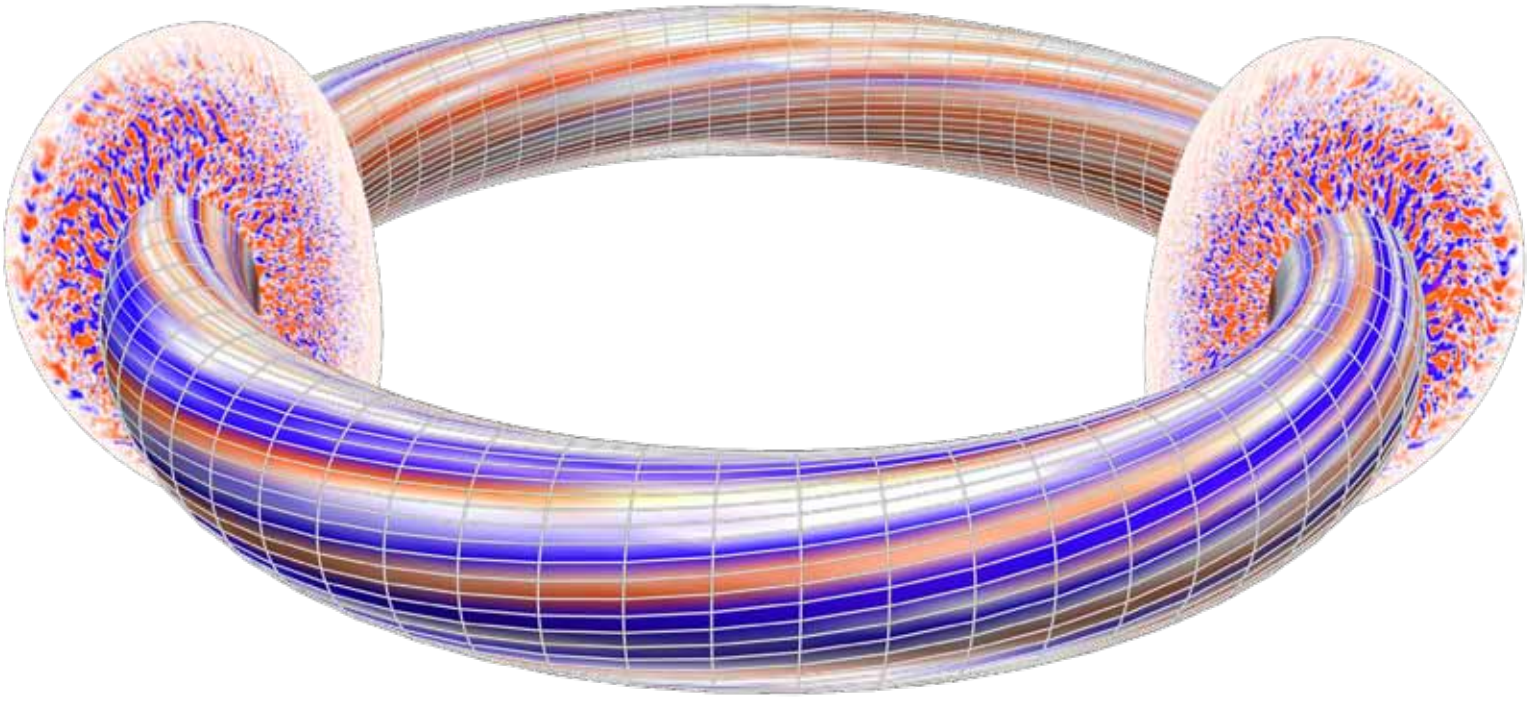
Fusion

Global Simulation of Plasma Microturbulence at the Petascale and Beyond

As the current global energy economy focuses on alternatives to fossil fuels, there is increasing interest in nuclear fusion, the power source of the sun and other stars, as an attractive possibility for meeting the world's growing energy needs. Properly understanding turbulent transport losses, which demands the application of computational resources at the extreme scale, is of the utmost importance for the design and operation of future fusion devices, such as the multi-billion dollar international burning plasma experiment known as ITER – a top priority investment in the Department of Energy's Office of Science. This Early Science project will achieve significantly improved understanding of the influence of plasma size on confinement properties in advanced tokamak systems such as ITER. This will demand a systematic analysis of the underlying nonlinear turbulence characteristics in magnetically confined tokamak plasmas that span the range from current scale experiments, which exhibit an unfavorable "Bohm-like" scaling with plasma size to the ITER scale plasma that is expected to exhibit a more favorable "gyro-Bohm" scaling of confinement. The "scientific discovery" aspect of such studies is that while the simulation results can be validated against present-day tokamaks, there are no existing devices today that are even one-third of the radial dimension of ITER. Accordingly, the role of high physics fidelity predictive simulations takes on an even more important role—especially since the expected improvement in confinement for ITER-sized devices cannot be experimentally validated until after it is constructed and operational. In dealing with this challenge, researchers will deploy GTC-P and GTS, which are highly scalable particle-in-cell gyrokinetic codes used for simulating microturbulence-driven transport in tokamaks.

Early Science Program Intrepid Allocation:

7.5 Million Hours



Fully kinetic 3-D plasma microturbulence simulation in a tokamak fusion device of the self-consistent electrostatic potential. The red and blue represent regions of positive and negative potential respectively. Elongated structures in the toroidal direction follow the magnetic field lines and is characteristic of the large anisotropy between the dynamics parallel and perpendicular to the magnetic field observed in tokamak experiments.

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Geophysics

Using Multi-scale Dynamic Rupture Models to Improve Ground Motion Estimates

Researchers will use Southern California Earthquake Center (SCEC) dynamic rupture simulation software to investigate high-frequency seismic energy generation. The relevant phenomena (frictional breakdown, shear heating, effective normal-stress fluctuations, material damage, etc.) controlling rupture are strongly interacting and span many orders of magnitude in spatial scale, requiring high-resolution simulations that couple disparate physical processes (e.g., elastodynamics, thermal weakening, pore-fluid transport, and heat conduction). Compounding the computational challenge, natural faults are not planar but instead have roughness that can be approximated by power laws potentially leading to large, multiscale fluctuations in normal stress. The capacity to perform 3-D rupture simulations that couple these processes will provide guidance for constructing appropriate source models for high-frequency ground motion simulations. SCEC's CyberShake system can calculate physics-based (3-D waveform modeling-based) probabilistic seismic hazard analysis (PSHA) curves for California.

On the next-generation Blue Gene, researchers, will calculate a 1Hz PSHA hazard map for California using improved rupture models from our multi-scale dynamic rupture simulations. They will calculate this high-resolution probabilistic seismic hazard map using the technique developed on the SCEC CyberShake project. This calculation will be done after integration of an improved pseudo-dynamic rupture generator into CyberShake system and production of a new and improved UCERF2.0-based Extended Rupture Forecast (ERF). The calculation will provide numerous important seismic hazard results, including a state-wide extended earthquake rupture forecast with rupture variations for all significant events, a synthetic seismogram catalog for thousands of scenario events, and more than 5,000 physics-based seismic hazard curves for California.

Early Science Program
Intrepid Allocation:
7.5 Million Hours

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Lattice Gauge Theory

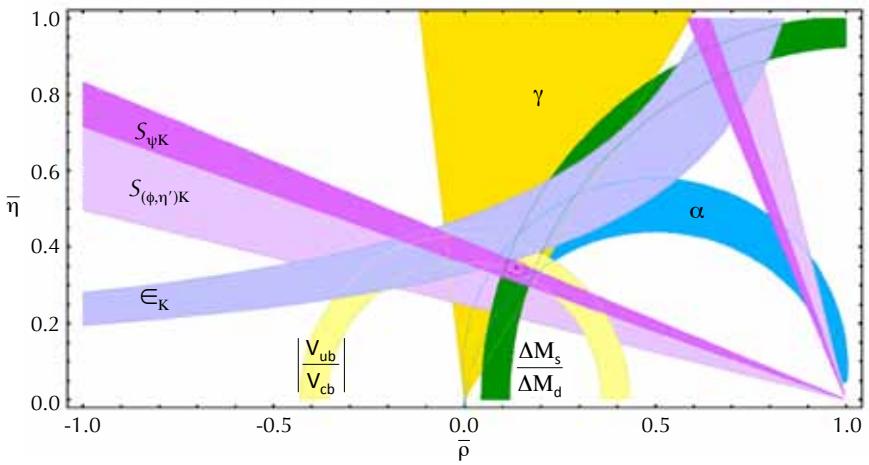
How Can We Better Understand the Basic Building Blocks of Nature?

Scientists have long sought to understand the basic building blocks of nature. While the behavior of particles such as protons and neutrons is well understood, less is known about the interactions of quarks and gluons, which compose them, the even-smaller particles that make up protons and neutrons. Because they interact very differently than larger particles, the study of interactions between quarks and gluons, Quantum Chromodynamics (QCD), requires different methodology. With the help of supercomputers, scientists use a four-dimensional lattice representation of space-time to analyze QCD.

This research aims to deepen the understanding of the interactions of quarks and gluons, the basic constituents of 99 percent of the visible matter in the universe. It will play a key role in ongoing efforts to develop a unified theory of the four fundamental forces of nature.

Scientists conducting QCD research have logged over 300 million core hours on the Blue Gene/P at the Argonne Leadership Computing Facility (ALCF). The scientists have generated gauge configurations with up, down, and strange quarks on lattices that are sufficiently fine-grained and have sufficiently small up and down quark masses to enable the extrapolation of key quantities to their physical values found in nature. The gauge configurations are being used to determine a wide range of important physical quantities in high energy and nuclear physics.

With the use of the Blue Gene/P, the generation of gauge configurations has been accelerated in many cases by a factor of 5 to 10 over what was previously possible with other machines.



The lattice QCD calculations performed of the decays and mixings of strongly interacting particles enable increasingly precise determinations of the parameters of the Standard Model of particle physics. This figure shows the bounds on the CP violating parameters rho *and* eta *obtained from the mixings of K and B mesons with their antiparticles and from the decay of a B meson into a pion plus leptons.*

Domain-wall configuration ensembles of lattice spacings 0.114 femtometers (fm) and 0.086 fm have been completed on lattices of sizes 24^3x64 and 32^3 x64, respectively. These are the largest domain-wall lattices ever attempted. For the staggered quarks, a set of runs with a lattice spacing of 0.06 and 0.045 fm have been completed. These are the most challenging staggered ensembles generated to date.

These ensembles are currently being analyzed at the ALCF and elsewhere in studies of the decays and mixings of particles containing heavy quarks to enable major improvements in determining a number of elements of the CKM matrix. These calculations are enabling precise tests of the Standard Model, aiding in a deeper understanding of fundamental physics.

Improved versions of both methods for lattice fermions are under way. For domain-wall fermions, a new method has been developed (the "AuxDet" method) that will permit a closer approach to the physical, light quark limit. For staggered fermions, an improved discretization method has been developed ("hisq" fermions) that substantially reduces discretization errors. New ensembles with the improved methods are expected soon.

INCITE Allocation:

67 Million Hours

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Materials Science

Interpreting IR Stretching Band of Liquid Water Improves Understanding of Hydrogen Bonding

In the last several decades, vibrational spectroscopy has been widely used to probe the structure and dynamics of water, and much progress has been made in the understanding of hydrogen bonding in the liquid, based on two-dimensional (2-D) IR spectroscopy. However, despite experimental and theoretical advances (e.g., the interpretation of IR and 2-D-IR spectra provided by several simulation studies), a detailed understanding of the infrared (IR) line shapes of liquid water has not yet been achieved.

University of California—Davis researchers interpreted the complex shape of the IR stretching band of neat, heavy water, using first principles molecular dynamics and *ab-initio* electronic structure calculations [1]. They carried out calculations using the Qbox code on Intrepid, the IBM Blue Gene/P supercomputer at the Argonne Leadership Computing Facility. The researchers showed that intermolecular dipolar correlations play a key role in determining the shape and width of the band, and that these correlations are long-ranged, extending to the second coordination shell. Both hydrogen-bonded and non-hydrogen-bonded molecules contribute to the IR stretching band over the entire frequency range, with no distinctive peak or shoulder associated with each species. Within a molecular orbital picture, the researchers identified specific features of the band arising from correlations of electronic contributions to the IR activity. The researchers' interpretation of the IR stretching band of water is providing a better understanding of hydrogen bonding. Additional spectroscopic investigations carried out by the UCD team, in collaboration with researchers at LLNL and MIT include the study of X-Ray absorption spectra [2].

Physics issues that remain to be explored include the effects of the presence of solvated ions on the properties of neat and confined water and the analysis of electronic spectra (e.g., x-ray absorption spectra).

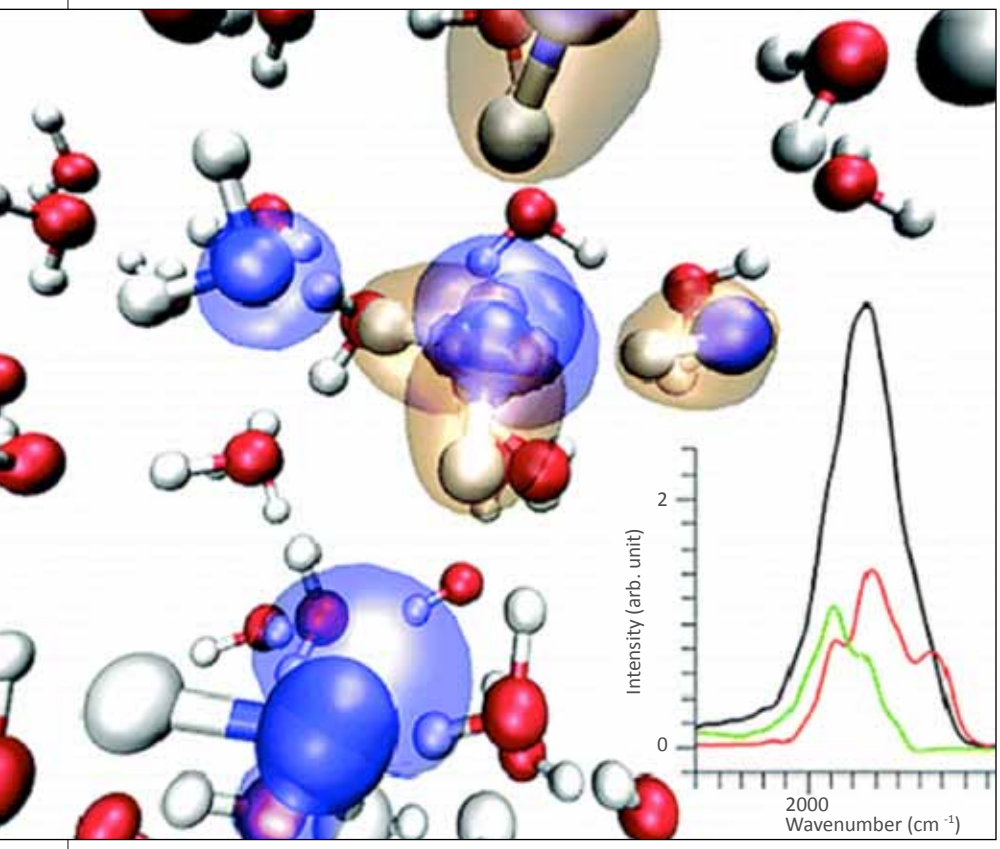
[1] "First Principle Analysis of the IR Stretching Band of Liquid Water", C. Zhang, D. Donadio and G. Galli, *J. Phys. Chem. Lett.*1, 1398 (2010).

[2] "Local Effects in the X-ray Absorption Spectrum of Salt Water", Heather J. Kulik, Nicola Marzari, Alfredo A. Correa, David Prendergast, Eric Schwegler, and Giulia Galli, *J. Phys. Chem. B* 114, 9594 (2010)

INCITE Allocation:

1 Million Hours

"The INCITE program has been very important in advancing our research, providing dedicated access to a high-performance computer managed by an extremely competent and helpful team."



Molecular orbital representation of the electronic states in the first solvation shell in water. The inset shows different contributions (total, inter- and intra-molecular) to the IR stretching band of liquid water.

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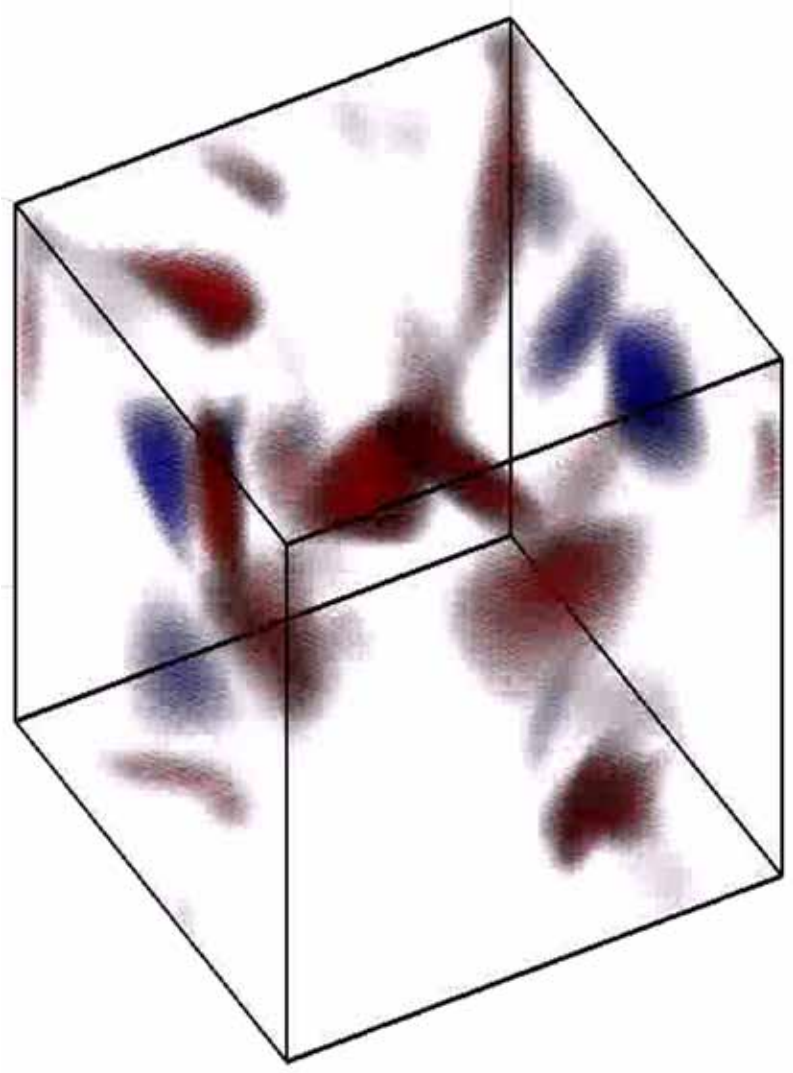
Materials Science

Large-Scale Condensed Matter and Fluid Dynamics Simulations

Identifying UPOs in the Navier-Stokes Equations with HYPO4D

University College London researchers are applying dynamical systems theory to three-dimensional fluid turbulence. They are taking a novel space-time variational approach using the HYPO4D code and have located several Unstable Periodic Orbits (UPOs). The main advantage of storing UPOs to represent a turbulent flow is that it needs to be done only once. In the future, the turbulent average of any given quantity can be computed directly from the UPO library with high accuracy and without the need to solve an initial value problem, using the dynamical zeta function formulation. This methodology has the potential to become a new paradigm in the study of large, driven dissipative dynamical systems, not only for the Navier-Stokes equations.

INCITE Allocation:
40 Million Hours



Snapshots of the vorticity field of a UPO located in weakly turbulent flow with Re=371 and period equal to 26864 LB time steps. The quantity shown is the magnitude of vorticity above a given cut-off level. Red corresponds to large negative vorticity (clockwise rotation), and blue to large positive vorticity (counter-clockwise rotation).

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University College London | p.v.coveney@ucl.ac.uk

Materials Science

Large-Scale Condensed Matter and Fluid Dynamics Simulations

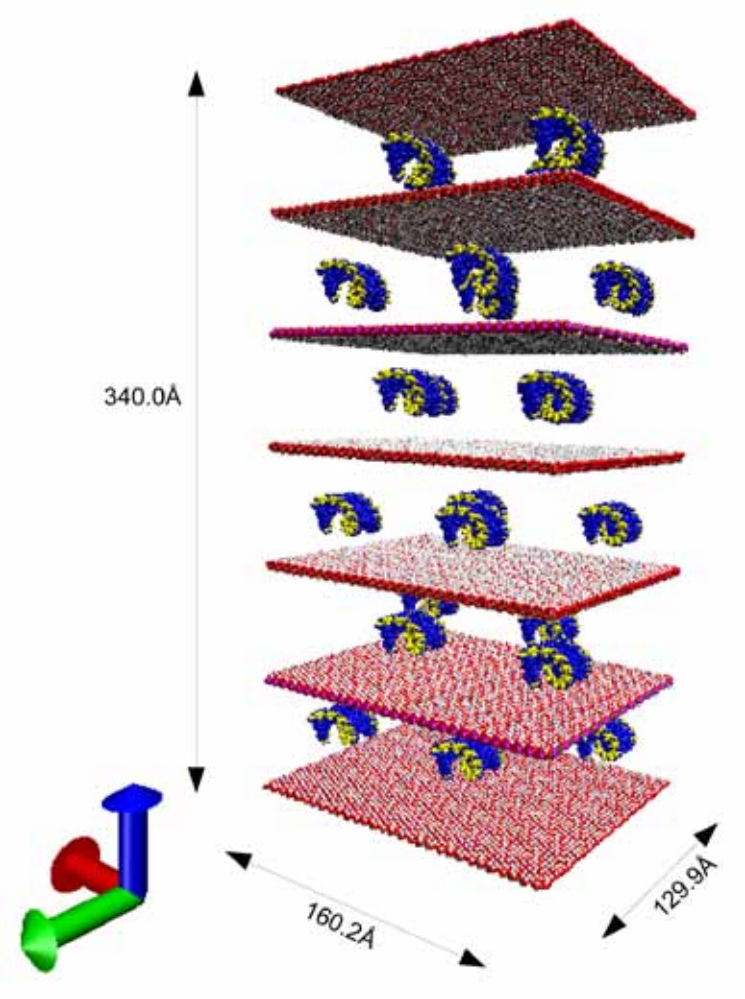
Conducting a Large-Scale MD Study of Clay-Polymer Nanocomposites

INCITE Allocation:
40 Million Hours

This work aims to investigate the complex interaction between clay-mineral systems and (bio-)polymers.

First, researchers at University College London are studying the physical and chemical aspects of clay platelets dispersed in a polymer matrix. Such nanocomposites have attracted widespread interest due to the improved properties they exhibit compared to their constituent parts; this is of great interest to the oil industry. Using replica exchange techniques on the IBM Blue Gene/P Intrepid at the Argonne Leadership Computing Facility allows the researchers to study systems 2-3 orders of magnitude larger than anything else currently published. Understanding the mechanisms by which clay platelets interact would be a major advance and may lead to rational design of materials with desired properties.

Second, they are studying the interactions of (bio-)polymers with clays. Such systems are relevant to origins of life studies. Research into the origins of life has rarely used simulation techniques to understand the possible chemical pathways to the formation of early bio-molecules. This work is providing insight into the structure, conformation, and stability of nucleic acids, while interacting with a clay surface and intercalated in the layered materials, which is extremely difficult to obtain accurately from experiments.



Initial stucture of the large LDH-nucleic acid models, (a) System, at the start of the simulation. For clarity, water molecules and chloride ions are not displayed. Magnesium, aluminum, oxygen, and hydrogen atoms within the LDH are represented as gray, pink, red, and white spheres, respectively; the atoms within the RNA phosphate backbone are shown as yellow spheres; and all other atoms within the RNA strands are represented as blue spheres.

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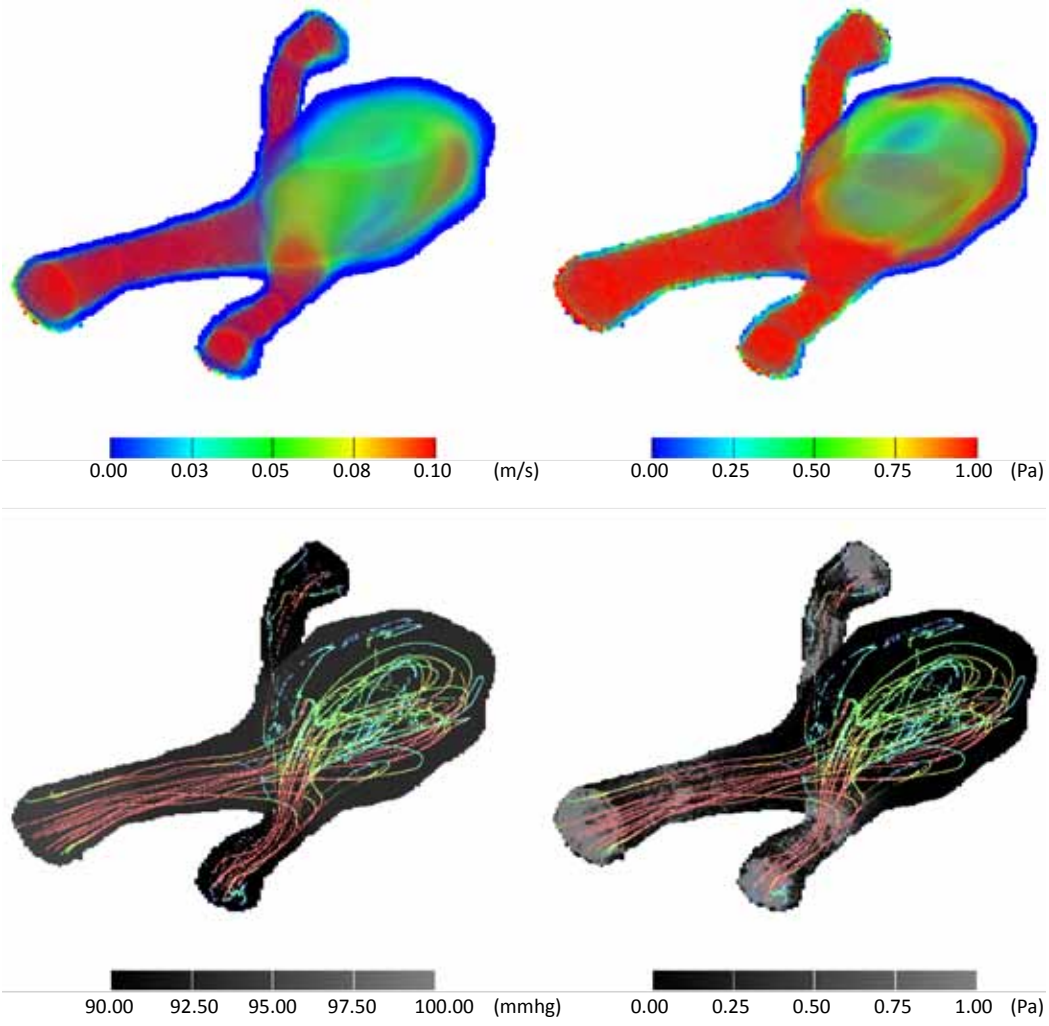
Materials Science

Large-Scale Condensed Matter and Fluid Dynamics Simulations

Simulating Brain Blood Flow to Better Diagnose, Treat Aneurisms

INCITE Allocation:
40 Million Hours

Patient-specific brain blood flow simulations are aiming to improve diagnosis and treatment of aneurisms. Researchers from University College London have made significant progress in studying three patients' internal carotid artery aneurysms. In conducting the simulations, the researchers used HemeLB, a sparse-geometry optimized lattice Boltzmann code, on Intrepid, the 557-teraflops IBM Blue Gene/P, at the Argonne Leadership Computing Facility. Intrepid allows flow calculation at speeds fast enough to be clinically useful. The simulations involved a number of steps—acquiring angiography data, transferring it to local resources, pre-processing locally, staging to remote resources for simulation, and reporting (using interactive steering and visualization).



A visualization of one aneurysm. Top Left: volume rendered velocity. Top Right: volume-rendered von Mises stress. Bottom Left: external pressure and streaklines. Bottom Right: external von Mises stress and streaklines.

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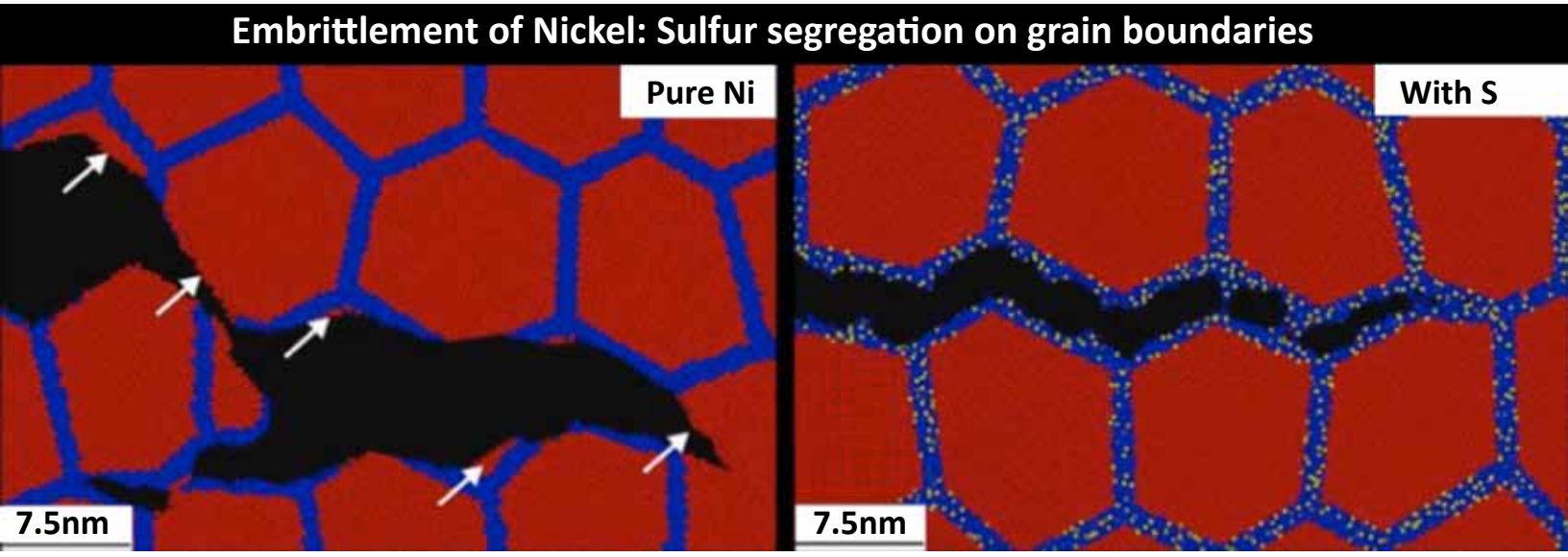
Materials Science

Modeling Nickel Fractures and Next-Generation Reactors

A multidisciplinary team of physicists, chemists, materials scientists, and computer scientists made innovations in simulation methods and parallel computing technologies to perform the largest-ever (48 million atoms), chemically reactive molecular dynamics simulation on 65,536 IBM Blue Gene/P processors at the Argonne Leadership Computing Facility. The team answered a fundamental question encompassing chemistry, mechanics, and materials science: How a minute amount of impurities segregated to grain boundaries of a material essentially alters its fracture behavior. The researchers simulated the introduction of small amounts of sulfur into the boundaries between nickel grains to investigate a material property known as "embrittlement." Seeing how different configurations of nickel function at these exceptionally small scales helps them understand the basic chemistry that will expedite the development of next-generation nuclear reactors. The study was published in *Physical Review Letters* (April 2010).

Director's Discretionary Allocation:

30 Million Hours



Closeups of fracture simulations for nanocrystalline nickel without and with amorphous sulfide grain-boundary phases, where red, blue, and yellow colors represent nickel atoms inside grains (>0.5 nanometers from grain boundaries), nickel atoms within 0.5 nm from grain boundaries, and sulfur atoms, respectively. The figure shows a transition from ductile, transgranular tearing to brittle, intergranular cleavage. White arrows point to transgranular fracture surfaces.

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Materials Science

Probing the Non-scalable Nano Regime in Catalytic Nanoparticles with Electronic Structure Calculations

To get insight into quantum-size effects (QSE) of nano-clusters and estimate the impact on their catalytic ability, Argonne researchers, in collaboration with colleagues at the Technical University of Denmark, performed Density Functional Theory (DFT) calculations on cuboctahedral gold clusters with adsorbed oxygen and carbon monoxide. The effective cluster sizes ranged from 0.5 to about 4 nm (13 to 1,415 atoms). The calculations were done on the IBM Blue Gene/P supercomputer at the Argonne Leadership Computing Facility. The researchers found the QSE to be energetically converged for clusters larger than 309 atoms – where they obtained the adsorption characteristics of single crystal surfaces. The QSE effects were on the order of 1 eV and had a huge impact on the estimated catalytic properties of the clusters. They also found the QSE to be essentially reproduced by a simple, tight-binding model with nearest-neighbor matrix elements estimated from bulk-gold calculations and fit to reproduce the adsorption characteristic of the single-crystal surfaces.

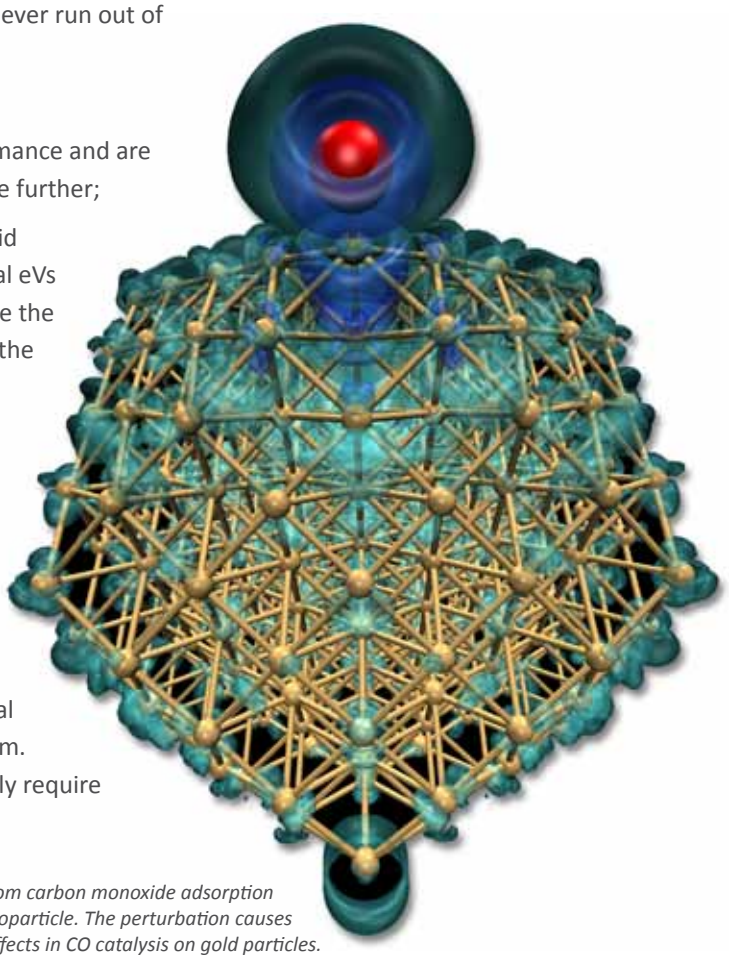
INCITE Allocation:
10 Million Hours

"The computational resources available through the INCITE program have permitted us to analyze the catalytic and electronic properties of nanoparticles that would have been impossible to study on more conventional systems."

Research accomplishments include:

- Completed parallelization of dense linear algebra—can now always run in VN mode with state-parallelization and will never run out of memory;
- Found new, efficient BG/P mappings;
- Did additional general tuning of the parallel performance and are working more closely with IBM to optimize the code further;
- Discovered a scheme that corrects for numerical grid effects (egg-box effect), which can sum up to several eVs for large systems – and which furthermore influence the relaxation of clusters (grid-snapping to hotspots of the egg-box effect).

Currently, the researchers are pursuing geometric relaxation of larger clusters and focusing their efforts on Pt and Rh, which, contrary to Au, have a partially filled d-band. They continue to work on integrating the HDF5 library into GPAW to allow the efficient restart of calculations using wave functions. They're also addressing a thorny technical challenge: Dense diagonalization arising from ScaLAPACK is one of several Amdahl limitations in the canonical O(N3) DFT algorithm. This is a non-trivial algorithmic bottleneck that will likely require implementing O(N) DFT algorithms as a resolution.



Electron density perturbation from carbon monoxide adsorption on a multi-hundred atom gold nanoparticle. The perturbation causes significant quantum size effects in CO catalysis on gold particles.

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Using Quantum Chemistry to Study Photocathodes

Ultra-thin MgO films on Ag(001) surfaces constitute an example of how ultra-thin surface layers on metals can be used to control the emittance properties of photocathodes. In addition to substantially reducing the work function of the metal surface, the MgO layers also favorably influence the shape of the surface bands, resulting in the generation of high-brightness electron-beams. As the number of MgO surface layers varies from 0 to 3, the emitted electron beam becomes gradually brighter, reducing its transverse emittance to 0.06 mm-mrad.

Collaborators from Argonne, Northern Illinois University, and the Illinois Institute of Technology are developing photocathodes with ultra-low transverse emittance—a prerequisite for the development of x-ray free-electron lasers and energy-recovery linac x-ray sources. These devices can be employed to obtain sharper images of single, large molecules, such as vital proteins in physiological solutions. The research will contribute to the creation of instruments that will enable the study of phenomena that are not experimentally accessible today, including those in the biological and environmental research sector.

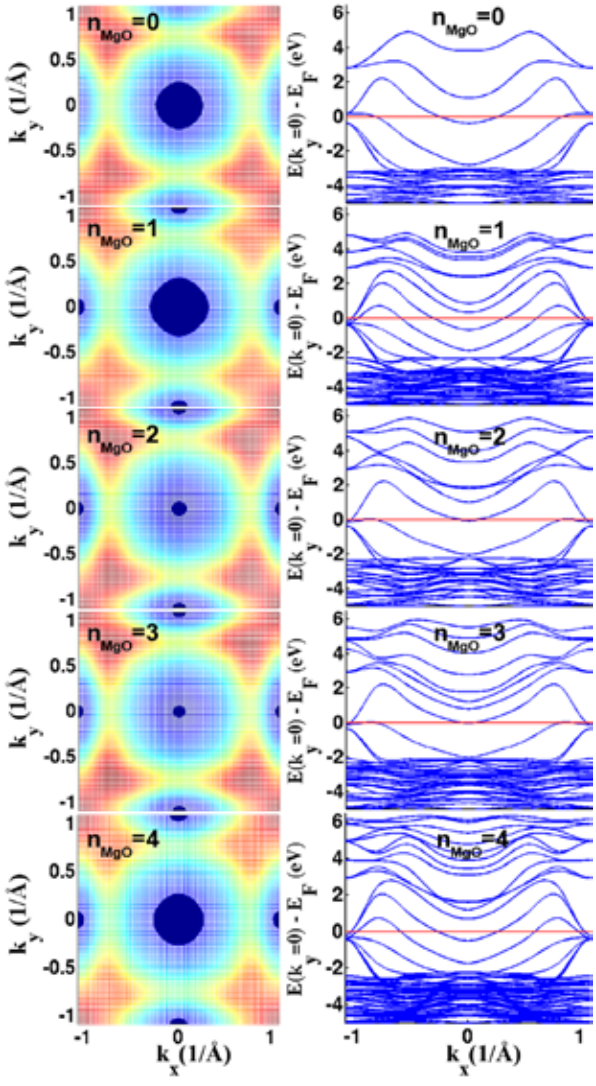
The research team is using the Quantum Espresso/PWSCF software package—a general quantum-mechanics code for atomic/molecular/solid-state physics and chemistry—to carry out the calculations of this work. The researchers are running their calculations on the Blue Gene/P at the Argonne Leadership Computing Facility and the Cray XT4 and XT5 at the National Energy Research Scientific Computing Center.

Researchers plan to conduct the screening of several other metal/oxide systems with the potential for low-transverse emittance photo-electrons by similar means. In addition, the team will study the effect of external electric field, surface roughness, etc. The best photocathode candidates will be tested experimentally.

Director's Discretionary Allocation:

0.5 Million Hours

"The Director's Discretionary Allocation has helped me to produce high-profile publications in the field of laser-plasma accelerators and photocathode research so far, and I expect to continue successful application of supercomputers in various fields of materials science, recently also in the analysis of x-ray scattering obtained of energy storage materials. The generous amounts of supercomputing time I have received helped me to quickly explore new ideas in the above-mentioned fields and elaborate research findings that proved to be the most promising directions."



Surface bands (left-hand panels) and the band structure (right-hand panels) of MgO(n_{MgO}ML)/Ag(001)(4ML)/MgO(n_{MgO}ML) systems in the Brillouin zone for n_{MgO}=0–4. Dark blue spots denote k-space regions with occupied electrons; otherwise, coloring indicates band height above E_F, the Fermi energy. Only surface bands with the highest energy occupied crystal orbitals in the center of the Brillouin zone are shown for each value of n_{MgO}.

Figure reproduced with permission from K. Nemeth et. al, Phys. Rev. Lett. *104, 046801 (2010).*

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Materials/Chemistry

Materials Design and Discovery: Catalysis and Energy Storage

This project targets four materials science problems that are critical to the Department of Energy's energy security mission: 1) biomass conversion, 2) electric energy interfaces, 3) lithium-air batteries, and 4) catalysis with high-Z metal nanoparticles. The first two of these are the impetus of the Energy Frontier Research Centers at Argonne National Laboratory: Institute for Atom-efficient Chemical Transformations and Center for Electrical Energy Storage. Lithium-air batteries are a Laboratory Directed Research & Development Director's Grand Challenge. Lastly, catalysis with high-Z metal nanoparticles is a major component of the ongoing research efforts at the Center for Nanoscale Materials. The computational method, Density Functional Theory (DFT), is the most frequently used electronic structure method because of its relative accuracy and favorable scaling with system size: O(N3). DFT has played an important role in understanding the properties of catalysts, electronic transport, spintronics, matter at extreme conditions, semiconductors, metals, and even BCS-type superconductors.

Early Science Program Intrepid Allocation:

3 Million Hours

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Nuclear Physics

Advancing the Understanding of Nuclear Structure

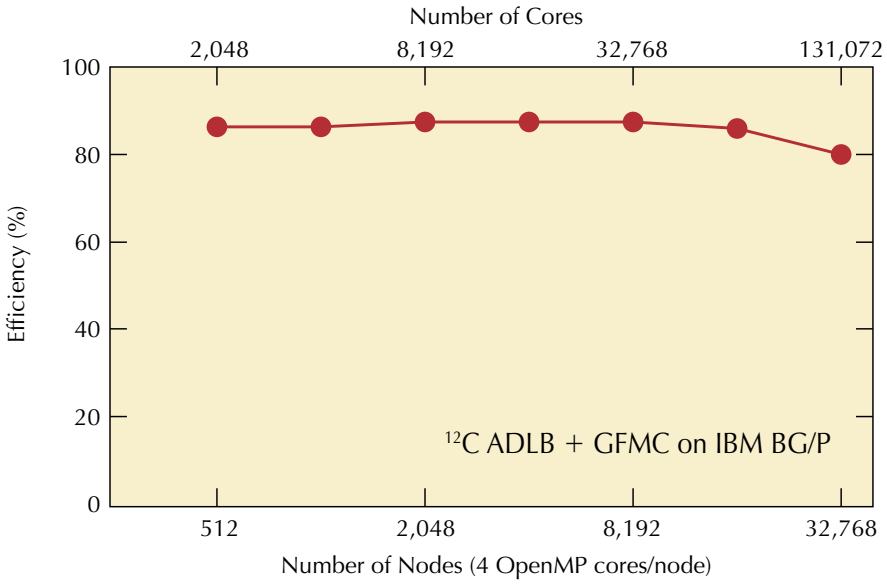
Researchers from Oak Ridge and Argonne national laboratories are using complementary techniques, including Green's Function Monte Carlo, the No Core Shell Model, and Coupled-Cluster methods to perform *ab initio* calculations of both structural and reaction properties of light- and medium-mass nuclei. The calculations use realistic models of nuclear interactions including both two- and three-nucleon forces. Their work could advance understanding of the triple-alpha burning reaction, which is essential to life on earth.

They also are exploring the role of the three-nucleon force in substantially heavier nuclei. Furthermore, researchers are using Density Functional Theory (DFT) to calculate properties of nuclei across the entire range of nuclear masses. These DFT studies will help predict nuclear properties relevant to nuclear reactions such as neutron-nucleus reaction cross-sections and fission. This new understanding of nuclei has far-reaching implications, impacting the fields of energy and astrophysics. The researchers are conducting their calculations on the IBM Blue Gene/P (BG/P) at the Argonne Leadership Computing Facility and the Cray XT at Oak Ridge National Laboratory.

The BG/P research team has completed ground-state ^{12}C calculations—a key milestone. The ground state represents the best converged *ab initio* calculations of ^{12}C ever. The researchers have continued developing and testing various formulations of starting wave functions for the first excited 0^+ state of ^{12}C (the Hoyle or triple-alpha burning state). While they have not yet found a starting wave function that remains orthogonal to the ground state wave function during Green's Function Monte Carlo (GFMC) propagation, this work is ongoing.

In order to enable the ^{12}C calculations on BG/P, computer scientists in Argonne's Mathematics and Computer Science Division developed the Asynchronous Dynamic Load Balancing library (ADLB), which provides GFMC with scalability in a simple work-sharing programming model. By using OpenMP on each node, the team is now getting essentially perfect scaling up to 65,536 nodes (32,768 are used for their production runs). The team is now using the ^{12}C GFMC calculations to test a new version of ADLB that uses the MPI one-sided puts and gets.

INCITE Allocation:
15 Million Hours



Excellent scaling is achieved by the production Automatic Dynamic Load Balancing (ADLB) library on the BG/P.

"The ^{12}C calculations require close to a million core hours each. This exploratory works requires many to be made; such resources are available only on the leadership-class machines."

Steve Pieper
Argonne National Laboratory

Contact ▸ David Dean
Oak Ridge National Laboratory | deandj@ornl.gov

Nuclear Structure

Ab-initio Reaction Calculations for Carbon-12

Researchers will calculate several fundamental properties of the 12C nucleus: the imaginary-time response, the one-body density matrix, and transition matrix elements between isospin- 0 and -1 states. These are needed to be able to reliably compute neutrino-12C scattering, which is needed for neutrino detector calibrations; quasi-elastic electron scattering, which is currently being measured at Jefferson Lab (JLab); and the results of older reactions on 12C.

In the past 15 years, researchers have developed Green's function Monte Carlo as a powerful and accurate method for computing properties of light nuclei using realistic two- and three-nucleon potentials. This will be the basis of all the calculations. Understanding the propagation of charges and currents in the nucleus is critical to a real understanding of the physics of nucleonic matter. Electron scattering experiments in the quasi- elastic regime, where the dominant process is knocking a single nucleon out of the nucleus, are under way at Jefferson Lab for a range of nuclei. The separation into longitudinal and transverse response allows one to study the propagation of charges and currents, respectively, in the nucleus. The nontrivial changes as one goes from the nucleon and deuteron to larger nuclei like carbon require one to consider processes well beyond simple, one-nucleon knockout. Researchers will compute the transition density matrices on a two-dimensional grid of the magnitudes of the initial and final positions. A partial wave expansion of the angle between the two vectors will be made.

Early Science Program
Intrepid Allocation:
7.5 Million Hours

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Nuclear Structure

Lattice Quantum Chromodynamics

Lattice quantum chromodynamics (LQCD) calculations are required to relate the experimentally observed properties of the strongly interacting particles to QCD, the fundamental theory of quarks and gluons. This research aims to produce the high-precision lattice QCD calculations that are urgently needed in the analysis of crucial experiments in high energy and nuclear physics that have recently been completed or are in progress. The broad aims of the calculations are to determine some of the basic parameters of the standard model of sub-atomic physics; to compute the masses, decay properties, and internal structure of strongly interacting particles; to obtain a quantitative understanding of the behavior of strongly interacting matter under extreme conditions of temperature and density; and to begin the study of strongly interacting theories that may be necessary to describe nature at the shortest distances.

Researchers will use the next-generation Blue Gene to generate gauge configurations that are representative samples of the systems being studied. These configurations will immediately be made available to all members of the U.S. Lattice Quantum Chromodynamics collaboration (USQCD), who will use them to perform a wide range of calculations. Members of USQCD are currently generating gauge configurations with three different formulations of lattice quarks, anisotropic clover, domain wall (DWF), and highly improved staggered quarks (HISQ), each of which has important advantages for different aspects of our work. Researchers expect to be using these formulations at the time of the Early Science Program. The next-generation Blue Gene will enable them to generate configurations that would support calculations of the spectrum, decay properties and internal structure of strongly interacting particles, and tests of the standard model, of unprecedented precision.

Early Science Program
Intrepid Allocation:
7.5 Million Hours

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Physics

Direct Multiobjective Optimization of Storage Ring Lattices for the APS Upgrade and Beyond

The brightest gets brighter

The brightest storage ring-generated x-ray beams in the Western Hemisphere are created by Argonne's Advanced Photon Source (APS) and are used by more than 5,000 scientists worldwide. A planned upgrade to the APS will reconfigure the facility's magnets (its "lattice") to enhance this world-class resource. The addition of long superconducting devices will increase brightness by an order of magnitude for x-rays above 20 keV. The upgrade will also accommodate systems for dramatically reducing the x-ray pulse length, giving the APS a unique position for enabling time-resolved science with hard x-rays. Without disruption to current operating modes, the upgrade will result in an improved source of high-energy, high-brightness, tunable x-rays for scientific research.

When massive compute power is elegant

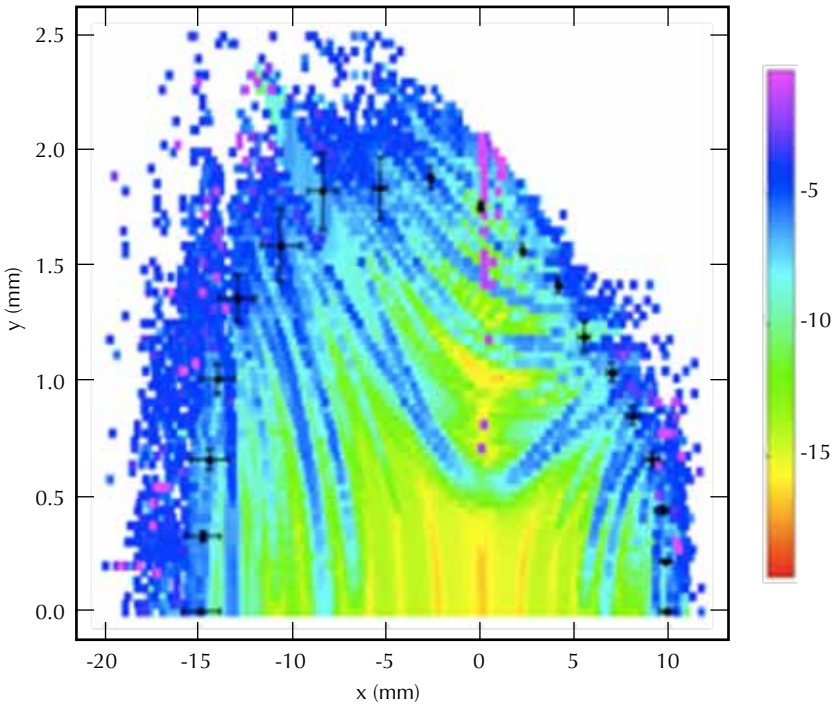
Scientists at work on the APS upgrade are challenged with optimizing the nonlinear dynamics to provide both sufficient dynamic aperture (to ensure high-injection efficiency) and momentum aperture (to ensure sufficient beam lifetime). To tackle this challenge, researchers will pair the extreme computing power of the ALCF's Blue Gene/P with the APS-developed code "elegant" to create complex particle-tracking simulations.

Providing faster solutions today, building resources for tomorrow

The vast compute power of the Blue Gene/P gives scientists at work on the APS upgrade the ability to resolve more challenging problems faster. To keep pace with the community's seemingly insatiable appetite for increased brightness, researchers will use a portion of their ALCC allocation to advance important concept work for next-generation "ultimate" storage rings.

ALCC Allocation:

36 Million Hours



Dynamic aperture for 50 error ensembles overlaid on frequency map for APS-U lattice with SPX and Reduced Horizontal Beamsize insertions. The optimization process successfully excludes strong resonances from the interior region.

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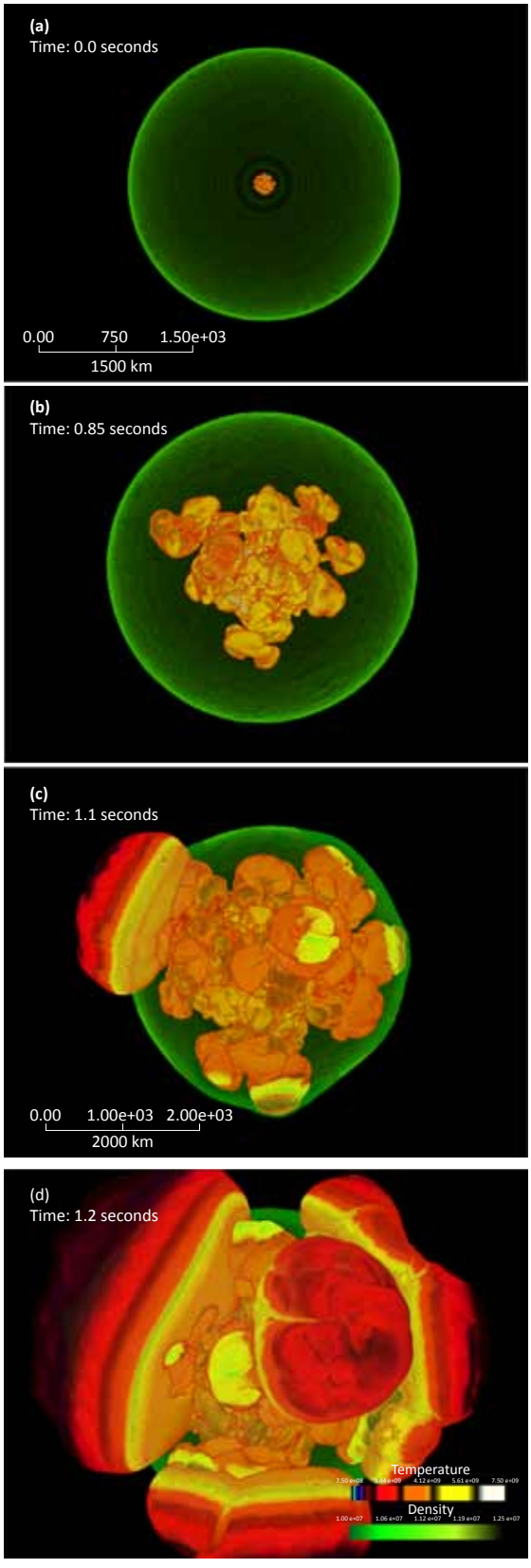
Physics

How Do Standard Candles Illuminate Knowledge of the Universe?



Type Ia supernovae (SNe Ia) are among the brightest exploding stars in the universe. Observations using SNe Ia as "standard candles" led to the discovery of dark energy. Most scientists believe that using SNe Ia to determine the properties of dark energy will require a much better understanding of these explosions.

Researchers are using the FLASH code and time on the IBM Blue Gene/P at the Argonne Leadership Computing Facility (ALCF) awarded through the U.S. Department of Energy's INCITE program to conduct the first comprehensive, systematic validation of current models of SNe Ia and to determine the fundamental properties of buoyancy-driven turbulent nuclear combustion – a physical process that is key to SNe Ia but is not fully understood.

The team has simulated all current models of Type Ia supernovae on the ALCF's Blue Gene/P. These simulations led to the discovery of robust signatures for the different SNe Ia models, holding out the promise that observations can discriminate among them. The team also has simulated buoyancy-driven turbulent nuclear combustion. These simulations show that the flame surface is complex at large scales and smooth at small scales, suggesting that the burning rate may be determined by the properties of the flame at large scales.

INCITE Allocation:

70 Million Hours

"The time awarded to the Center under the INCITE program has been essential to the team's ability to achieve these scientific results."

Four snapshots during a simulation of the explosion phase of the deflagration-to-detonation (DDT) model of nuclear-powered (Type Ia) supernovae. The images show extremely hot matter (ash or unburned fuel) and the surface of the star (green). Ignition of the nuclear flame was assumed to occur simultaneously at 63 points randomly distributed inside a 128-km sphere at the center of the white dwarf star. The images show volume renderings of extremely hot regions and the surface of the star [defined as the region in which the density is (1.0 - 1.25) x 10^{7} g cm^{-3}]. (a): 0.0 seconds, showing the initial distribution of ignition points. (b): 0.85 seconds, when the bubbles have become Rayleigh-Taylor unstable and developed into mushroom shapes on their way to the surface of the star. (c): 1.1 seconds, when the first plume of hot ash has made its way to the surface, and the flame front has entered the distributed burning regime, initiating a detonation. (d): 1.2 seconds, after several plumes of hot ash have reached the surface and multiple detonations have occurred, while the first detonation wave is propagating through the star. Images were created from a simulation run on the Blue Gene/P at the Argonne Leadership Computing Facility in 2009.

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Physics

Nucleon Structure Down to the Physical Pion Mass

First-ever calculation of nucleon structure using full lattice QCD at the physical pion mass

Researchers led by John Negele from MIT's Center for Theoretical Physics will use their ALCC allocation to perform the first calculation of nucleon structure using full lattice QCD at the physical pion mass. Working with the Budapest-Marseille-Wuppertal (BMW) collaboration and using their 2+1 flavor dynamical stout-smeared O(a)-improved Wilson quark configurations for nucleon structure observables, they will calculate connected diagram contributions to form factors, moments of structure functions, and generalized form factors at 6 pion masses from approximately 338 MeV down to the physical pion mass at lattice spacing ~ 0.12 fm.

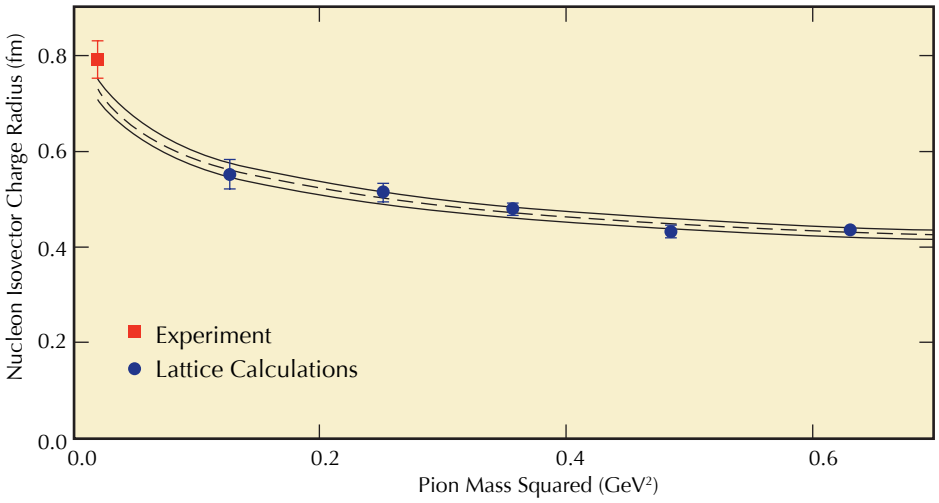
The team will study scaling behavior by calculating observables for m ~ 250 MeV at a ~ 0.12, 0.09, and 0.07 fm and finite volume corrections effects by comparing results for mL = 4.1 and 5.5 at m = 296 MeV. They will also conduct an extensive calculation of disconnected quark diagrams and gluon contributions for m ~ 250 MeV at a ~ 0.12 fm.

Optimized code, exceptional performance

The software for the stout-smeared O(a)-improved Wilson fermion calculations was optimized by Stefan Krieg for the Blue Gene/P. At these lattice sizes, the Dirac operator achieves a maximum of 37 percent of peak and typically runs at approximately 32 percent of peak on one to sixteen racks. The full inverter runs at more than 32 percent of peak. Using their own optimized domain wall inverter, performance is exceptional and provides significant advantage to the U.S. lattice QCD effort of international QCD software development supported by ASCR and NNSA.

ALCC Allocation:

37.8 Million Hours



Fundamental properties of the nucleon, such as the charge radius shown here, can be calculated from first principles by solving QCD numerically on a space-time lattice. This figure shows results featured in the DOE NSAC long-range plan, which had to be extrapolated from the left-most blue point to the physical pion mass shown in red. The goal of the current project is to calculate the radius at several masses lower than the lightest blue point as well as at the physical pion mass, to remove any extrapolation ambiguity.

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Physics

Simulating Laser-Plasma Interactions in Targets for the National Ignition Facility and Beyond

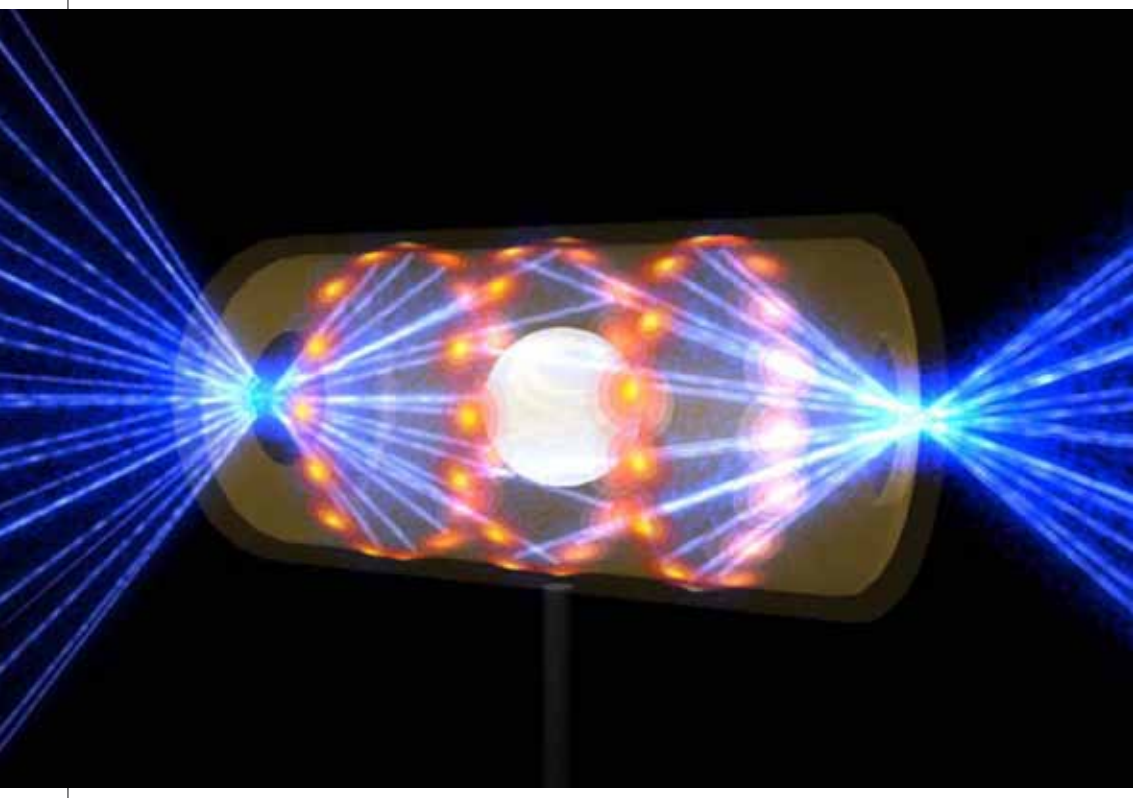
Lawrence Livermore National Laboratory (LLNL) has been tasked with achieving ignition at the National Ignition Facility (NIF). An important aspect of the ignition campaign involves quantitative prediction of the level of laser backscatter in these targets. Mitigation of laser backscatter is important, as backscatter reduces the amount of input energy available for driving the fusion process. It can also alter implosion symmetry as well as preheat the ignition capsule via generation of hot electrons.

Recent experimental results from the National Ignition Campaign at NIF show that backscatter occurs in the laser target where quads of laser beams are overlapped. The goal of these simulations is to quantify how overlapping beam quads impact laser backscatter. In the first simulation completed, which ran on the full BG/P Intrepid machine at Argonne, three quads of NIF beams propagated 750 micrometers, through half of the interaction region where laser backscatter occurs (113 billion zones). The beams were not polarization smoothed, a technique used at NIF to reduce laser backscatter. (Simulating the full backscatter region or including polarization smoothing results in a simulation too large for the full Intrepid machine.) Laser backscatter primarily occurs in the left and right beam quads because the resonance region for the central beam quad is marginally included in this simulation.

The simulations being conducted by LLNL researchers will generate scientific results that will have a major impact on the national ignition campaign—inertial fusion—as well as on the fundamental science of LPI. These state-of-the-art simulations are only possible because of the INCITE award received on the ANL BGP Intrepid machine.

INCITE Allocation:

45 Million Hours



NIF Hohlraum. This artist's rendering shows a NIF target pellet inside a hohlraum capsule with laser beams entering through openings on either end. The beams compress and heat the target to the necessary conditions for nuclear fusion to occur. Ignition experiments on NIF will be the culmination of more than 30 years of inertial confinement fusion research and development, opening the door to exploration of previously inaccessible physical regimes. Credit: Lawrence Livermore National Laboratory.

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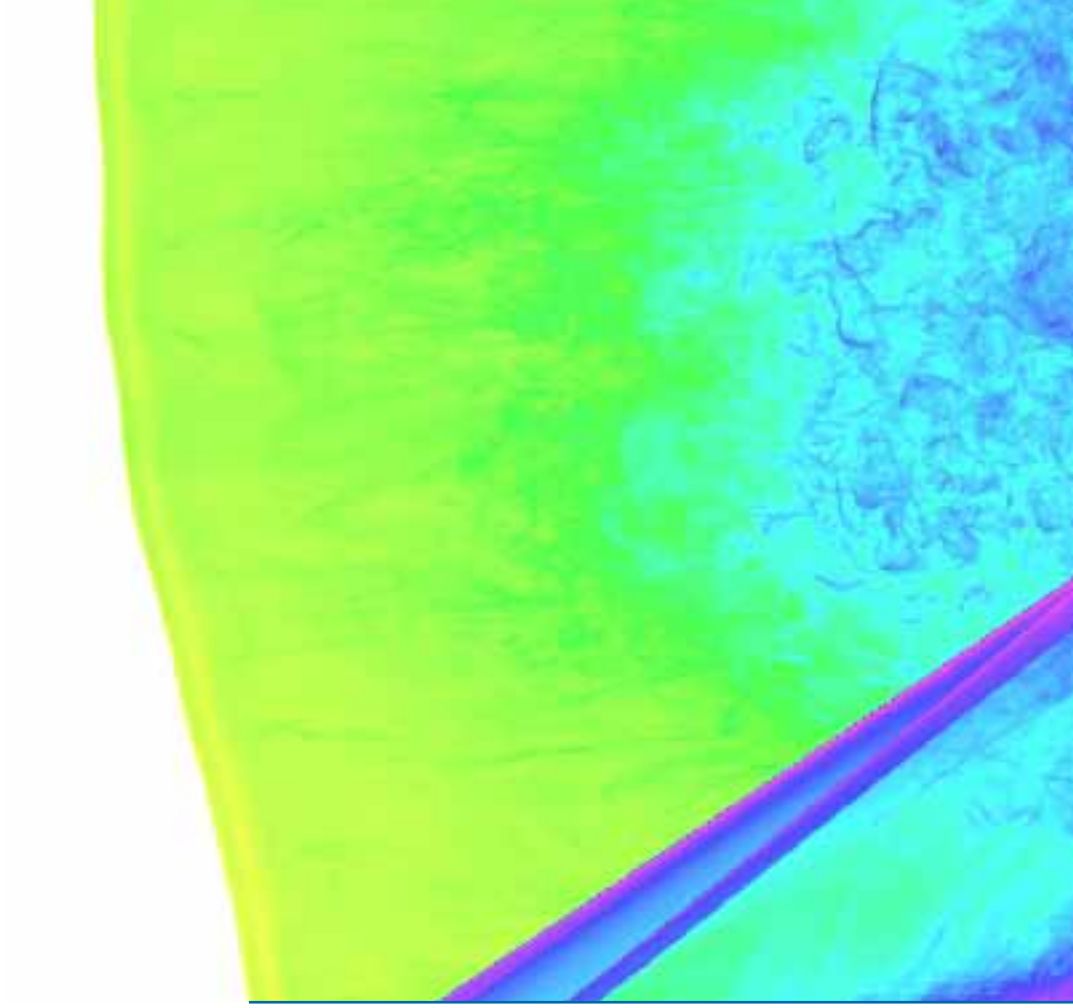

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